Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary materials

In silico study of structure and water dynamics in CNT/Polyamide nanocomposite reverse osmosis membranes

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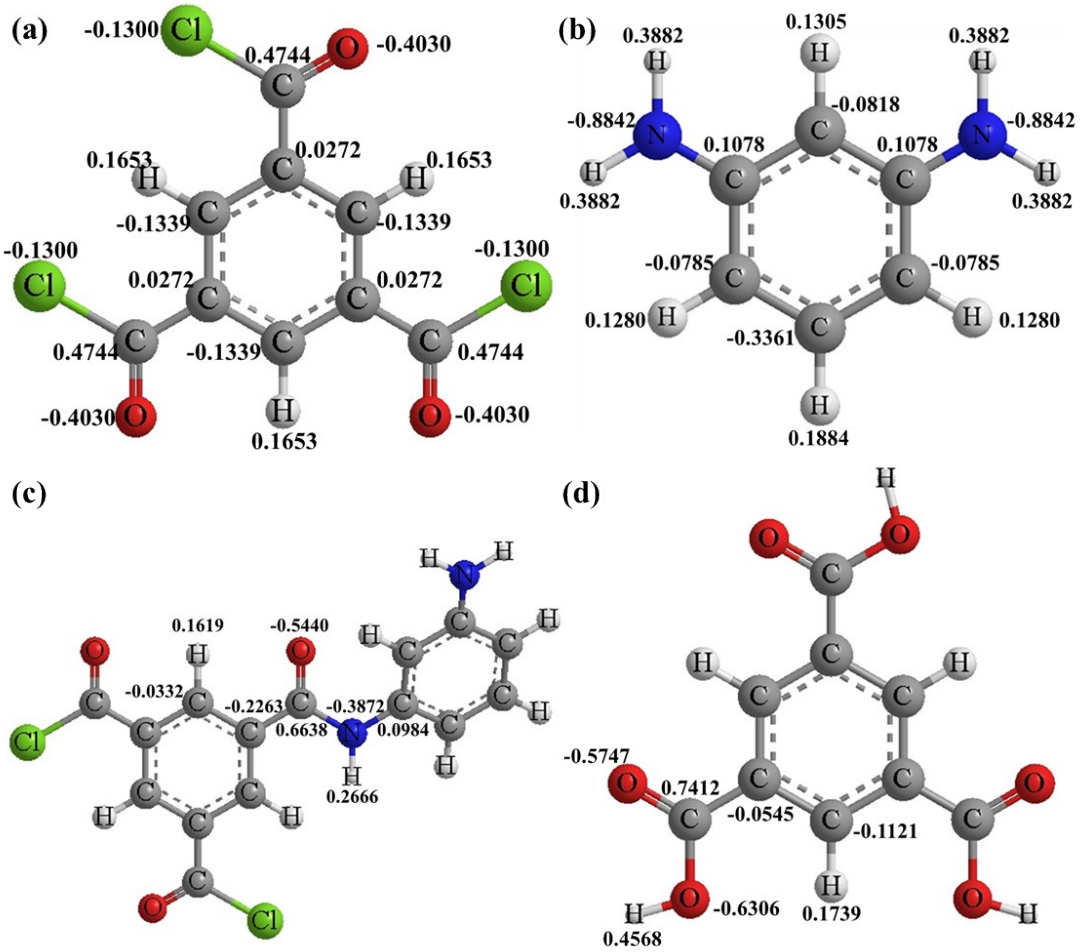

Fig. S1 (a) Partial charge assignment of TMC. (b) Partial charge assignment of MPD. (c) Change in partial charge assignment when an amide bond is formed. (d) Change in partial charge assignment after hydrolyzation. All the partial charges were calculated by RESP software.

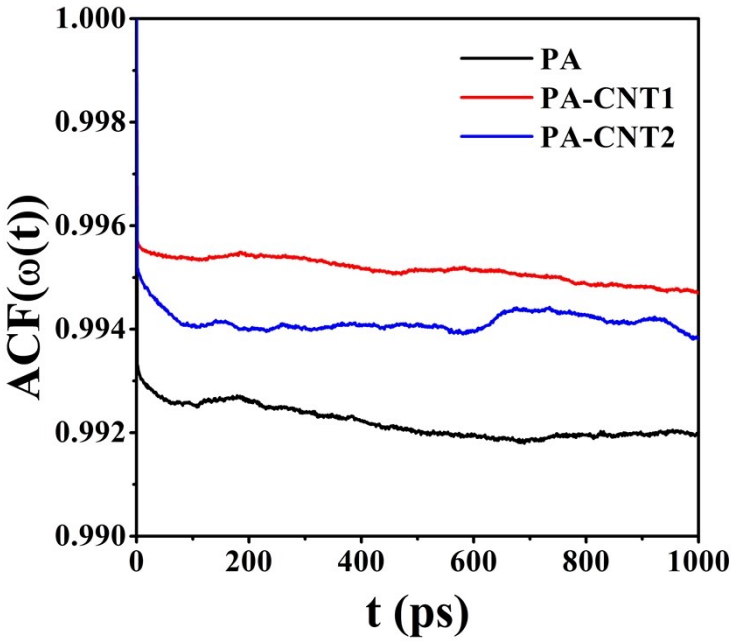

Fig. S2 Autocorrelation function of dihedral angle ω in hydrated PA, PA-CNT1 and PA-CNT2.

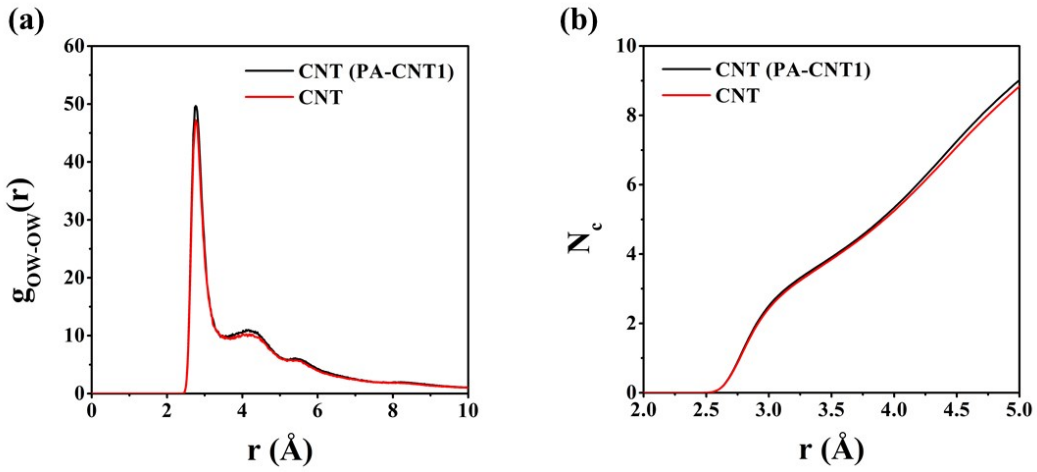

Fig. S3 (a) Radial distribution functions between oxygen atoms of water inside the CNT in PA-CNT1 and inside the plain CNT. (b) Coordination number of water molecules (N_c) inside CNT. N_c was calculated from the integration of the radial distribution functions in (a).

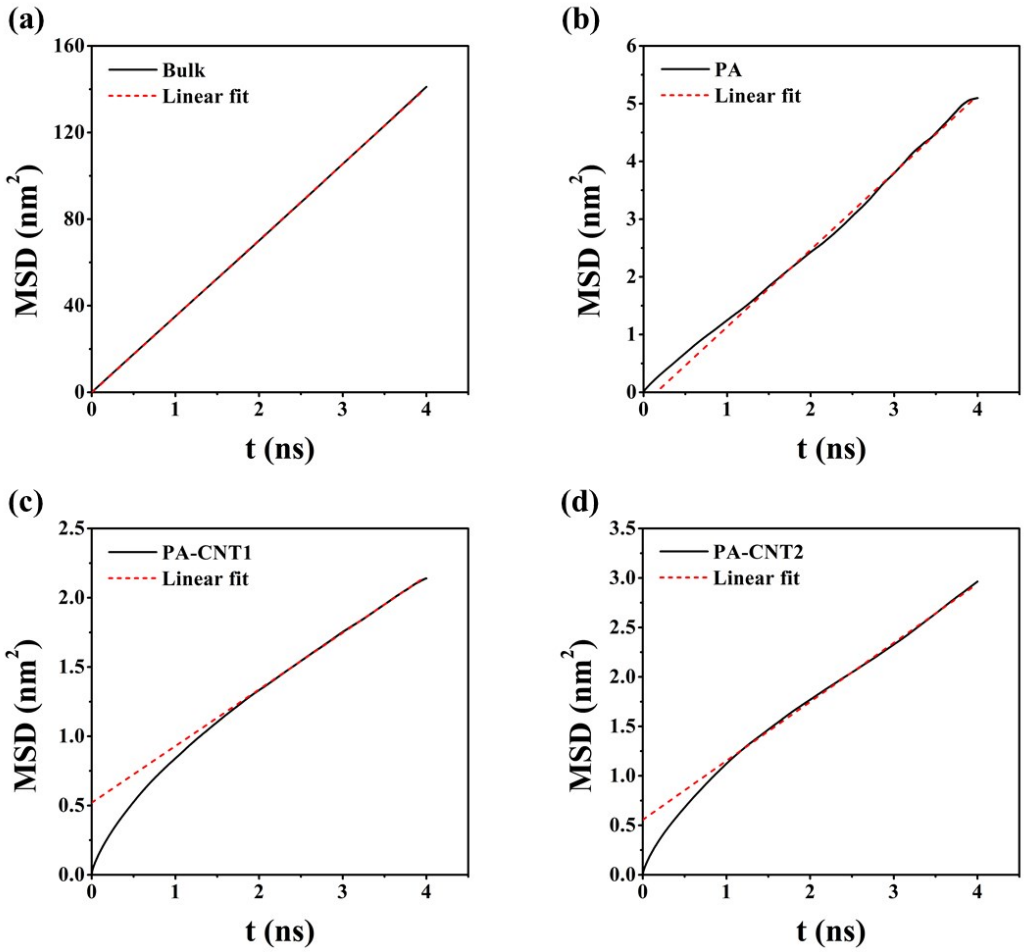

Fig. S4 Mean square displacement of water molecules and its linear fitting in bulk (a), in PA (b), in PA-CNT1 (c) and in PA-CNT2 (d).

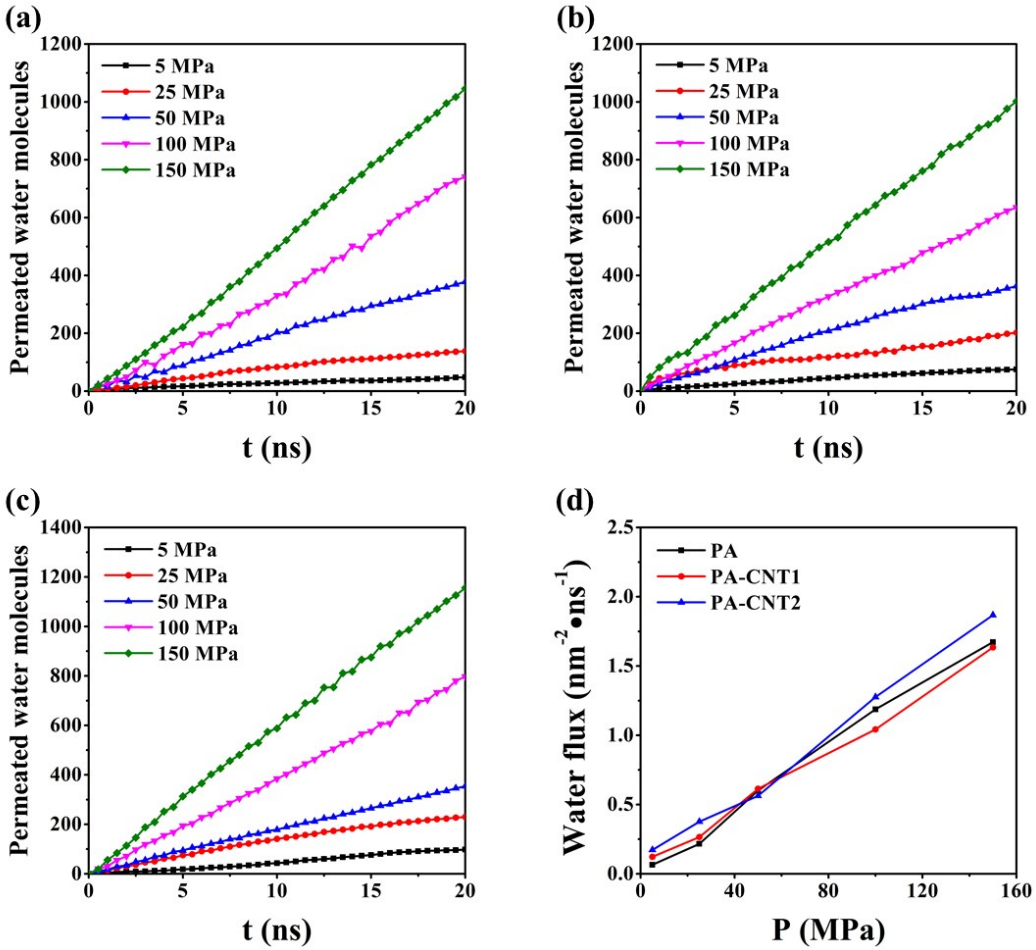

Fig. S5 The number of water molecules permeated through the membrane of PA (a), PA-CNT1 (b) and PA-CNT2 (c) as a function of time. (d) Water flux as a function of pressure in PA, PA-CNT1 and PA-CNT2.