Supplementary materials

Surface modification of polyamide reverse osmosis membrane with small-molecule zwitterions for enhanced fouling resistance: a molecular simulation study

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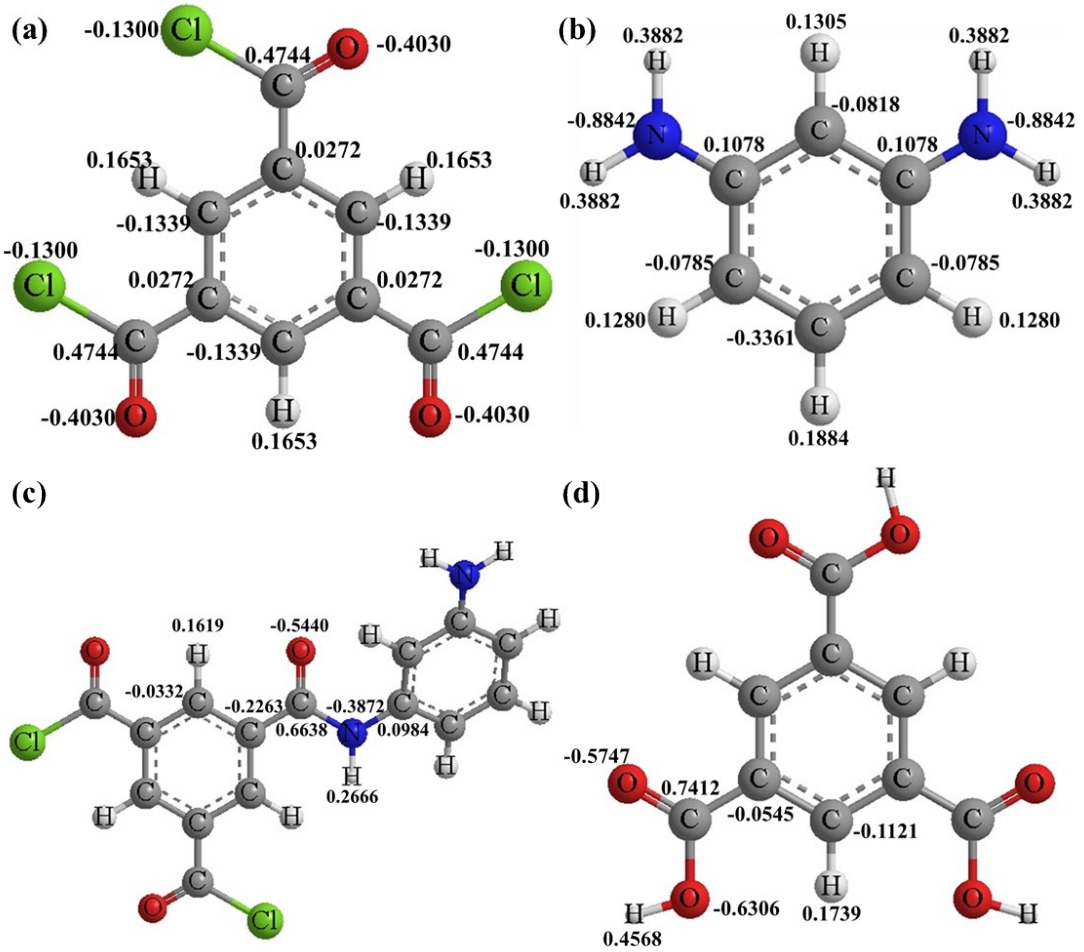

Fig. S1 (a) Partial charge assignment of TMC. (b) Partial charge assignment of MPD. (c) Change in partial charge assignment when an amide bond is formed. (d) Change in partial charge assignment after hydrolyzation. All the partial charges were calculated by RESP software.

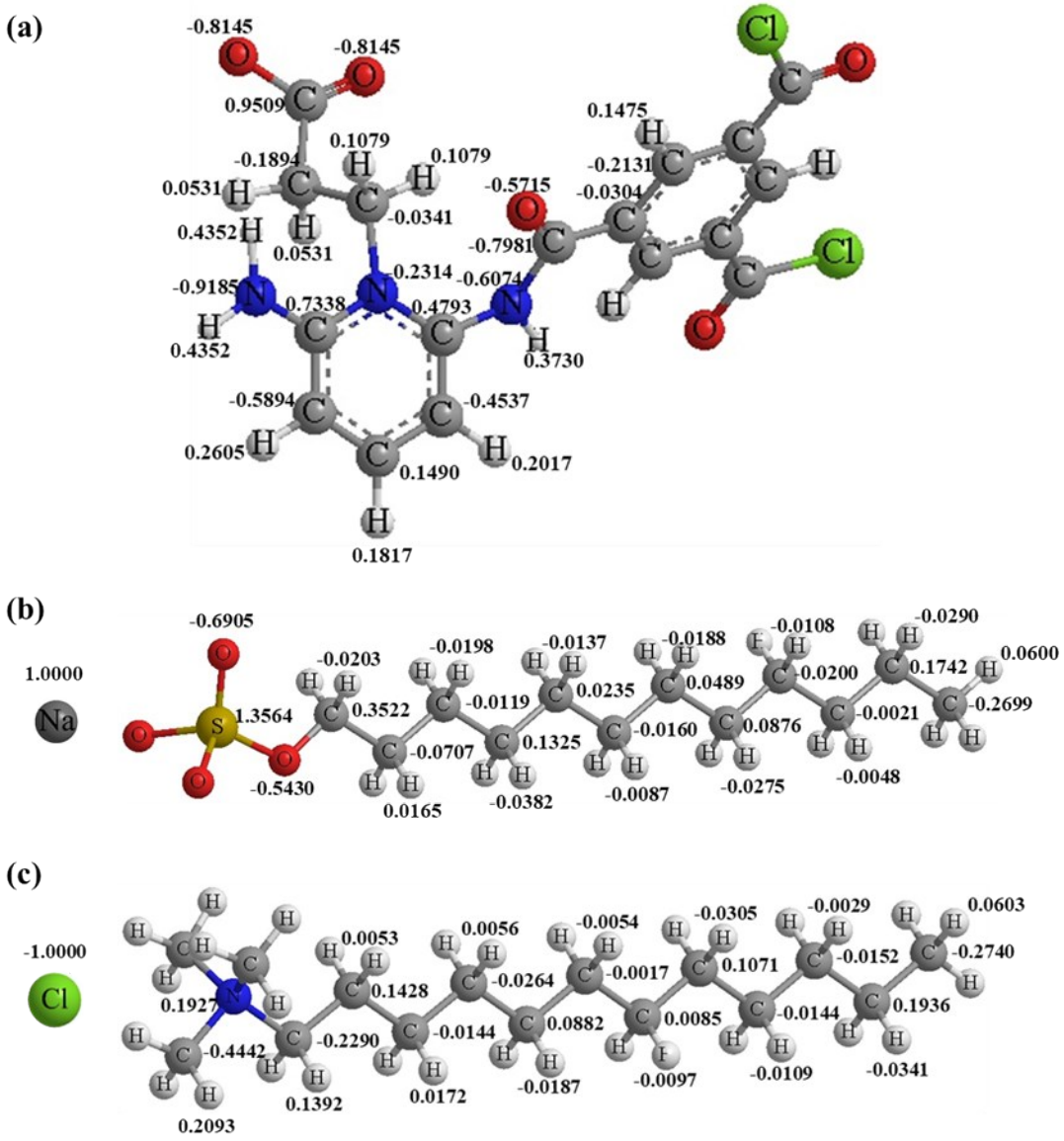

Fig. S2 (a) Change in partial charge assignment when an amide bond is formed between TMC and QDAP. (b) Partial charge assignment of SDS. (c) Partial charge assignment of DTAC.

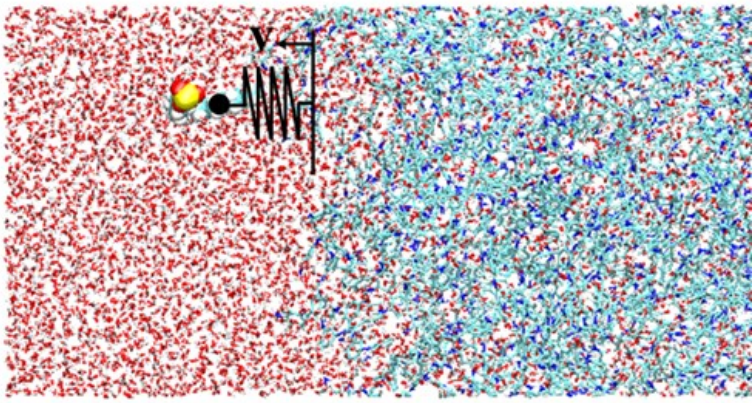

Fig. S3 VMD illustration of umbrella sampling, where water molecules are colored with red, polyamide is colored with cyan and SDS is represented with vdW sphere.

Umbrella Sampling:

The basic principle of umbrella sampling, taken the desorption of SDS from the membrane surface in PA as an example, is shown in Fig. S3. The conformation that SDS was adsorbed to the membrane surface was set as the initial conformation. A force was applied to the center of mass of the foulant so that it could be desorbed and move into the reservoir. The magnitude of the force changed every moment to keep the velocity of desorption maintained 0.1 nm·ps^{-1}. A series of conformations were then recorded with a 0.2 nm spacing of the distance d. For each conformation, the whole system was equilibrated for 10 ns under constant pressure. Then, a force was applied to the center of mass of the foulant, whose magnitude changed every moment so that the velocity of the foulant could maintain 0. After 10 ns simulation, the magnitude of the force and the distribution of the distance d were traced so that the PMF could be calculated using formula as follows: $PMF(d) = -k_B T ln[P(d)]$, where k_B is the Boltzmann constant, T is the temperature of the system and $P(d)$ is the probability distribution over 10 ns of the distance d between the foulant defined with its center of mass and the membrane surface. The distributions of the distance d in all conformations were then reconstructed by the reweighting method so that a continuous curve of PMF can be thus generated.