

## Supporting Information

Evaluation of proton transport and solvation effect in hydrated Nafion membrane with  
degradation

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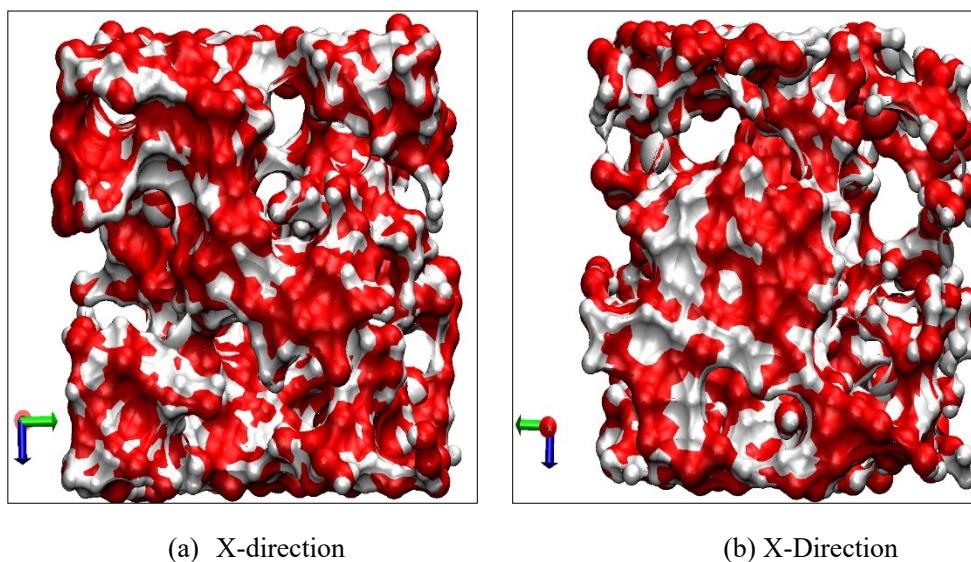
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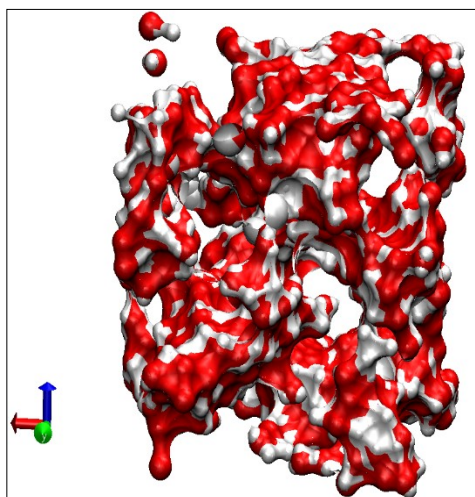
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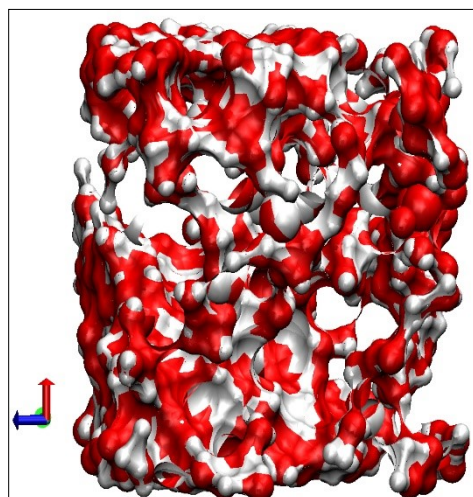
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Fig. S1 Snapshots of hydrophilic domains along the X/Y/Z direction in the hydration Nafion membrane at  $\lambda=15$ . (a) (c) (e) without attack (b) (d) (f) with attacked C-S bond (O in water-red, H in water-white)

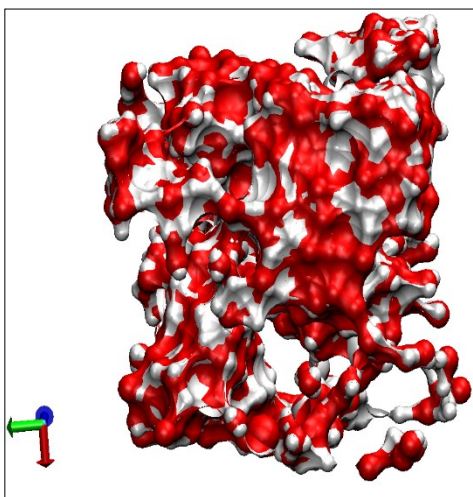




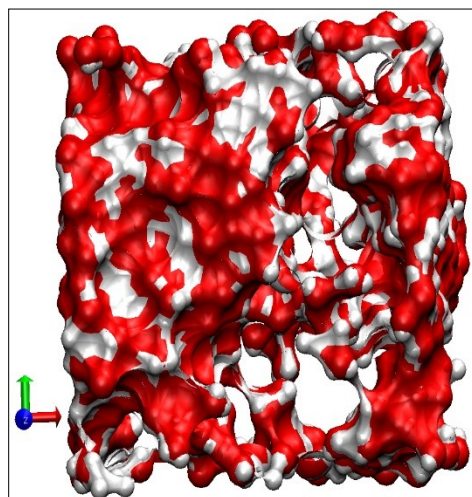
(c) Y-Direction



(d) Y-Direction



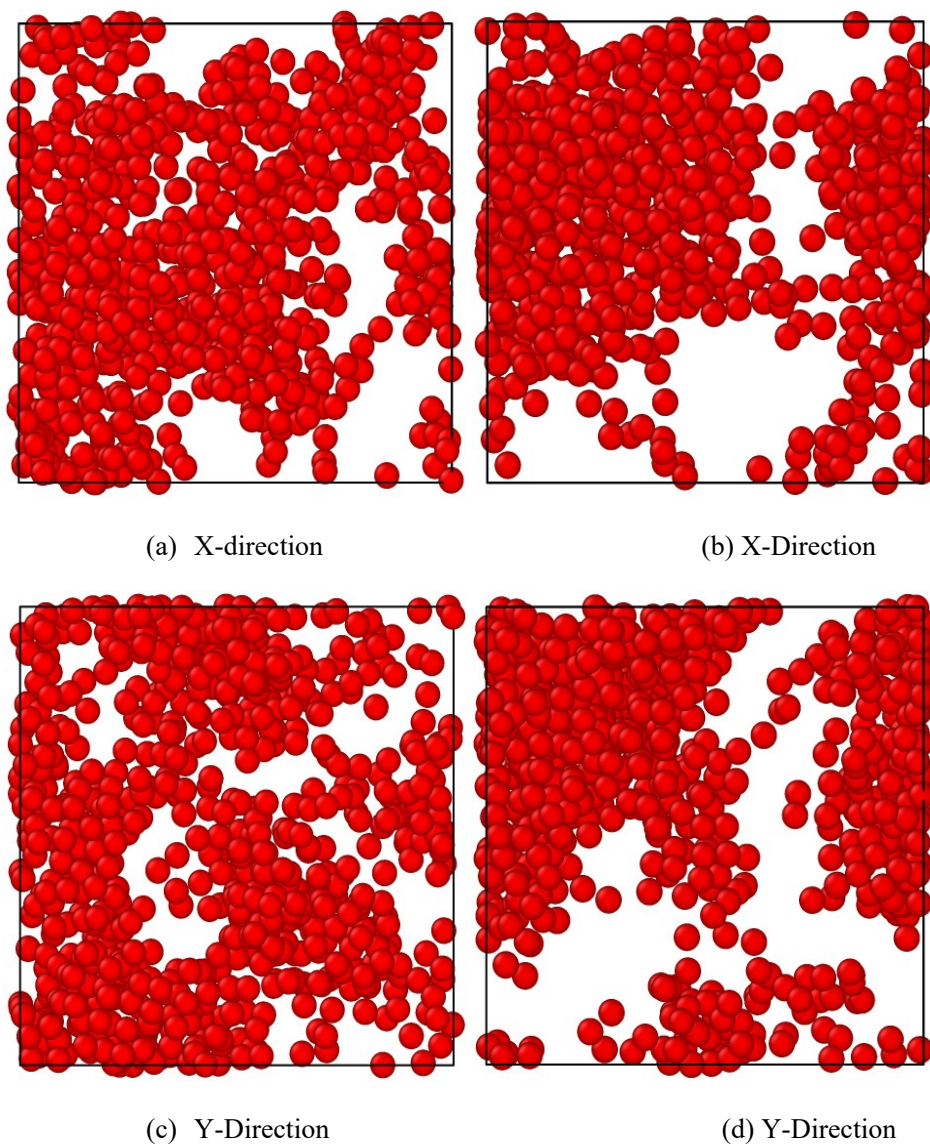
(e) Z-Direction



(f) Z-Direction

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Fig. S2 Snapshots of the largest hydrophilic clusters along the X/Y/Z direction in the hydration Nafion membrane at  $\lambda=15$ . (a) (c) (e) without attack (b) (d) (f) with attacked C-S bond (O in water-red)





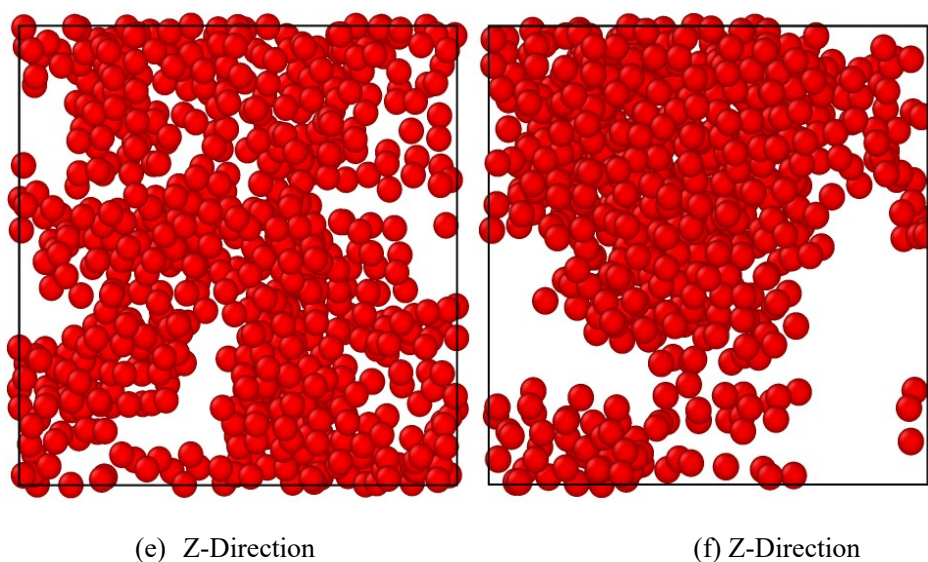
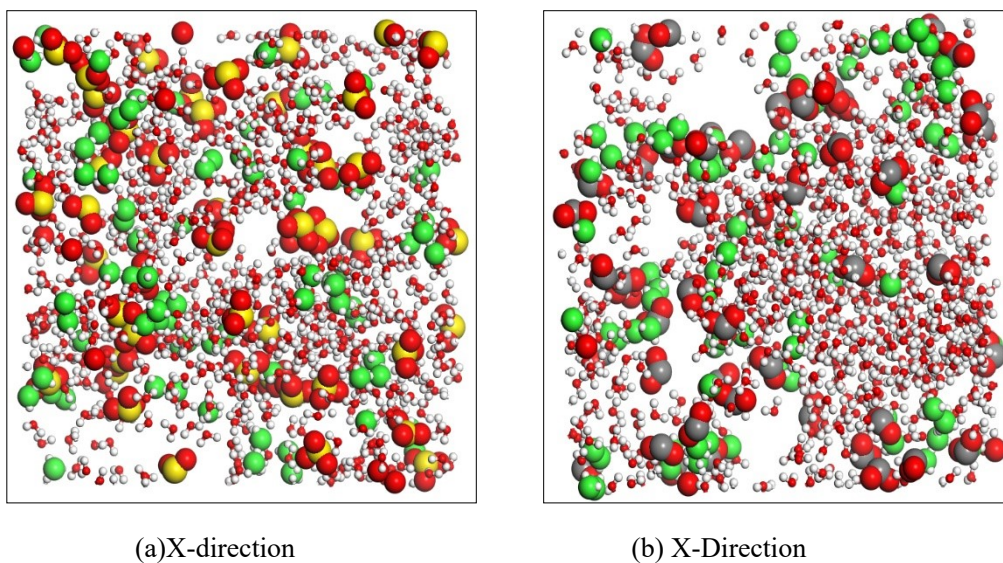
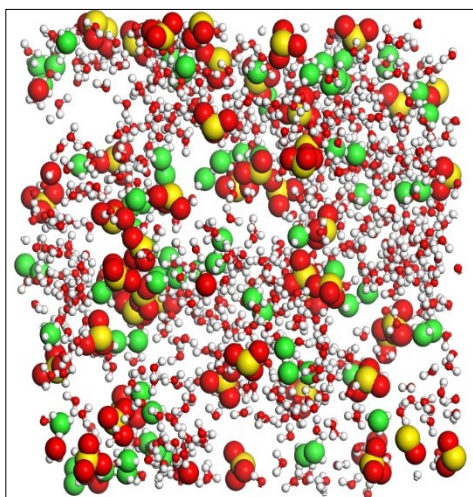
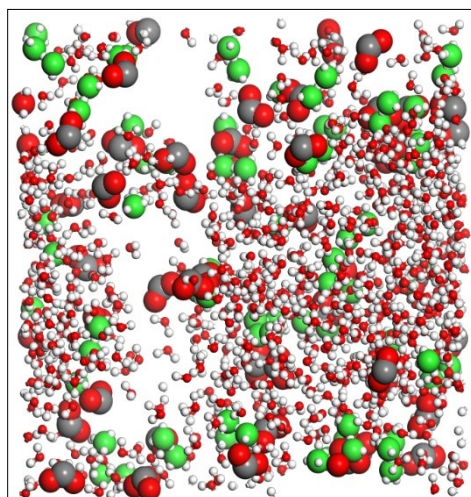


Fig. S3 Snapshots of hydronium ion and sulfonic acid/ carboxylic acid group distribution atoms along the X/Y/Z direction in the hydrated Nafion membrane with  $\lambda = 15$ . (a) (c) (e) without attack, (b) (d) (f) with attacked C-S bond (O atom in water-red, H atom in water-white, O atom in hydronium ion-green and magnified, H atom in hydronium ion-white, S and O atom in sulfonic acid group-yellow and red with magnified, C and O atom in carboxylic acid group-grey and red with magnified)

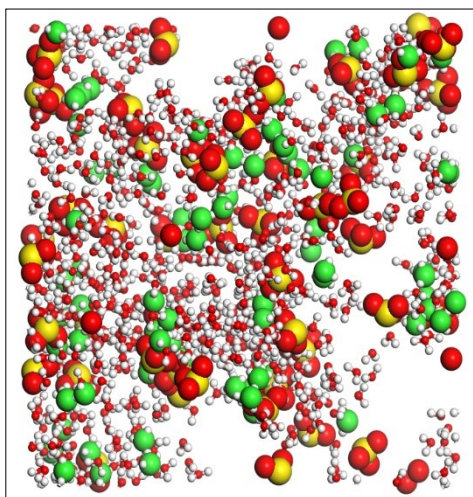




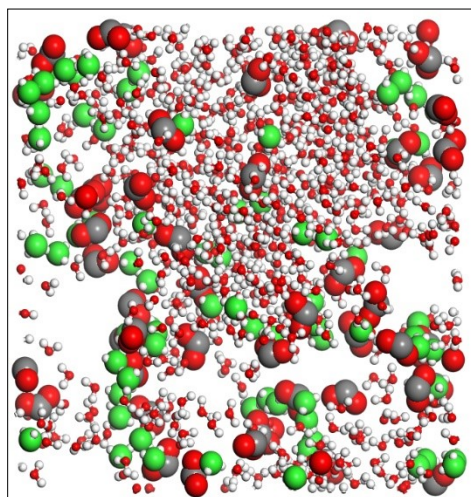
(c) Y-Direction



(d) Y-Direction



(e) Z-Direction



(f) Z-Direction