Increasing the proton conductivity of sulfonated polyether ketone by incorporating graphene oxide: Morphology effect on proton dynamics

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We synthesized graphene oxide–sulfonated polyether ether ketone (GO–SPEEK) composite membrane and compare its proton conductivity with that of Nafion®117 and SPEEK membranes. From experimental measurements, we found that GO–SPEEK has better proton conductivity ($\sigma^{\text{GO-SPEEK}}$ = 3.8 x 10^{-2} S cm^{-1}) when compared to Nafion®117 (σ^{Nafion} = 2.4 x 10^{-2} S cm^{-1}) and SPEEK (σ^{SPEEK}= 2.9 x 10^{-3} S cm^{-1}). From density functional theory (DFT-) based total energy calculations, we found that GO–SPEEK has the shortest proton diffusion distance among the three membranes, yielding the highest tunneling probability. Hence, GO–SPEEK exhibits the highest conductivity. The short proton diffusion distance in GO–SPEEK, as compared to Nafion®117 and SPEEK, can be attributed to the presence of oxygenated functional groups of GO in the polymer matrix. This also explains why GO–SPEEK requires the lowest hydration level to reach its maximum conductivity. Moreover, we have successfully shown that the proton conductivity σ is related to the tunneling probability T, i.e., $\sigma = \sigma' \exp(-1/T)$. We conclude that the proton diffusion distance and hydration level are the two most significant factors that determine the membrane's good conductivity. The distance between ionic sites of the membrane should be small to obtain good conductivity. With this short distance, lower hydration level is required. Thus, a membrane with short separation between the ionic sites can have enhanced conductivity, even at low hydration conditions.