Electronic Supplementary Information *for*

Nature of Proton Conduction in a Polymer Electrolyte

Membrane, Nafion

*Yoong-Kee Choe¹, Eiji Tsuchida¹, Tamio Ikeshoji¹, Shunsuke Yamakawa², Shi-Aki Hyodo²

¹Research Institute for Computational Sciences (RICS), National Institute of Advanced Industrial Science and Technology (AIST), Centeral-2, Umezono 1-1-1, Tsukuba, Ibaraki 305-8578, Japan. ²Toyota Central R&D Labs., Inc., Nagakute, Aichi, 480-1192, Japan.

*Corresponding author : <u>yoongkee-choe@aist.go.jp</u>

Fig. S1 shows mean square displacement (MSD) of proton (positive charge defect). It is seen that after 1 ps, MSD increases virtually linearly, which indicates that statistics are reasonably collected for the evaluation of diffusion coefficient.

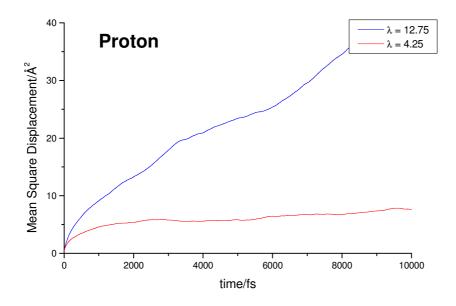


Fig. S1. Mean square displacement vs. time for proton