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Molecular Dynamics Simulation of Polysulfone-Based Anion Exchange Membrane Fuel Cell SEUNG SOON JANG, KYUNG WON HAN, JI IL CHOI, School of Materials Science and Engineering, Georgia Institute of Technology, 771 Ferst Drive NW, Atlanta, GA 30332-0245, COMPUTATIONAL NANOBIO TECHNOLOGY LABORATORY TEAM — In this study, we investigate the nanophase-segregated structures and transport properties of quaternary ammonium grafted polysulfone membranes using molecular dynamics simulation method. For this, we develop a new force field from a reference density functional theory modeling with B3LYP and 6-31G** in order to describe the hydroxide anion. The bond stretching force constant is determined to reproduce the quantum mechanical vibrational frequency. The atomic charges are determined by Mulliken population analysis. Through the annealing procedure, the nanophase-segregated structure is developed as a function of water contents such as 10 and 20 wt %. The extent of nanophase-segregation is evaluated by the structure factor analysis, which can be compared with the experimental small angle scattering data. Once the equilibrium structures are obtained, we run long MD simulations to analyze the diffusion of water and hydroxide using the mean-square displacement analysis with an assumption of Gaussian diffusion. The nanophase-segregated structures and the transport properties will be compared to the proton exchange membrane consisting of the same polymer backbone except for the acidic functional group.

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