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Effect of Temperature on Nanophase-segregation and Transport in Polysulfone-Based Anion Exchange Membrane Fuel Cell: Molecular Dynamics Simulation Approach KWAN HO KO, KYUNG WON HAN, Georgia Institute of Technology, School of Mechanical Engineering, JI IL CHOI, Georgia Institute of Technology, School of Materials Science and Engineering, YING CHANG, CHULSUNG BAE, Rensselaer Polytechnic Institute, Department of Chemistry and Chemical Biology, SEUNG SOON JANG, Georgia Institute of Technology, School of Materials Science and Engineering, GEORGIA TECH TEAM, RPI TEAM — The effect of temperature on hydrated polysulfone-based anion exchange membrane is studied using molecular dynamics. Various temperature conditions such as 313K, 353 K and 393K with two different water contents (10 wt % and 20 wt %) are simulated. From the viewpoint of structure-property relationship, we scrutinize the change in the nanophase-segregated structure of membrane and transport of anionic charge carrier (hydroxide) as a function of temperature. Since it is well known that the anion transport is less than the proton transport, we attempt to pursue a fundamental understanding of the difference between anion transport and proton transport. For this purpose, we simulate the polysulfone-based proton exchange membrane that has the same molecular structure and molecular weight. By analyzing the pair-correlation of charge carriers, we observe the correlation among hydroxides is much stronger than that among hydroniums. The extent of nanophase-segregation is also analyzed using structure factor profile.

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