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Study of Structural Behavior and Proton Conductivity of Inorganic Gel Paste Electrolyte at Various Phosphorous to Silicon Ratio by Multiscale Modelling

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Abstract : In polymer electrolyte membrane fuel cells (PEMFC), the membrane electrode assembly (MEA) is consisting of two platinum coated carbon electrodes, sandwiched with one proton conducting phosphoric acid doped polymeric membrane. Due to low mechanical stability, flooding and fuel cell crossover, application of phosphoric acid in polymeric membrane is very critical. Phosphorous and silica based 3D inorganic gel gains the attention in the field of supercapacitors, fuel cells and metal hydrate batteries due to its thermally stable highly proton conductive behavior. Also as a large amount of water molecule and phosphoric acid can easily get trapped in Si-O-Si network cavities, it causes a prevention in the leaching out. In this study, we have performed molecular dynamics (MD) simulation and first principle calculations to understand the structural, electronics and electrochemical and morphological behavior of this inorganic gel at various P to Si ratios. We have used dipole-dipole interactions, H bonding, and van der Waals forces to study the main interactions between the molecules. A 'structure property-performance' mapping is initiated to determine optimum P to Si ratio for best proton conductivity. We have performed the MD simulations at various temperature to understand the temperature dependency on proton conductivity. The observed results will propose a model which fits well with experimental data and other literature values. We have also studied the mechanism behind proton conductivity. And finally we have proposed a structure for the gel paste with optimum P to Si ratio.

Keywords : first principle calculation, molecular dynamics simulation, phosphorous and silica based 3D inorganic gel, polymer electrolyte membrane fuel cells, proton conductivity
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