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GIST discovers a way to improve the performance of high-temperature polymer membrane fuel cells

- GIST (Gwangju Institute of Science and Technology, President Kiseon Kim) School of Materials Science and Engineering Professor Jae-Suk Lee and Professor Joo-Hyoung Lee along with Graduate School of Energy Convergence Professor Chanho Pak confirmed that the functional groups* in a polymer electrolyte membrane had an effect on the outflow of phosphoric acid** and presented a method to improve the performance of high-temperature polymer membrane fuel cells.

  * functional group: a functional group is a specific group of atoms or bonds within a compound that is responsible for the characteristic chemical reactions of that compound

  ** phosphoric acid: a compound consisting of phosphorus (P), 4 oxygen (O), and 3 hydrogen (H) atoms that is acidic and moves hydrogen ions in a high-temperature polymer membrane fuel cell

  - The research team not only minimized the outflow of phosphoric acid by optimizing the functional groups in the electrolyte membrane and also investigated the phenomenon of phosphoric acid outflow through computational science, and this is expected to be used in the future to develop fuel cells for next-generation buildings with high efficiency.

□ High-temperature polymer membrane fuel cells that operate at temperatures above 120 degrees are attracting attention as a next-generation building-type fuel cell system because they have the advantage of using waste heat for hot water and heating. The fuel cell moves hydrogen ions through phosphoric acid in the electrolyte membrane, but during the operation of the fuel cell, phosphoric acid leaks from the electrolyte membrane to the electrodes, resulting in poor performance of the fuel cell.

□ The research team prepared and compared a polymer electrolyte membrane with three different azole compounds* introduced to investigate the phenomenon of phosphoric acid leakage. The azole compound is relatively basic compared to phosphoric acid, so it is possible to contain phosphoric acid in the electrolyte membrane through acid group interaction. In addition, the effect of nitrogen substituent and basicity of the azole compounds substituted with hydrogen and methyl groups** on phosphoric acid leakage from the electrolyte membrane was studied.

* azole compound: compounds containing atoms other than carbon atoms in the five-membered ring and containing at least one nitrogen atom

** methyl group: a compound in which one hydrogen atom of methane (CH_4) is removed and joined to the functional group of an azole compound

◦ The best performance (0.197 W/cm^2) was confirmed as a result of applying methyl imidazole* electrolyte membrane (6.9% outflow), which had a small amount of phosphoric acid leakage when the electrolyte membrane containing phosphoric acid was exposed to moisture. In addition, by calculating the bonding force between phosphoric acid, azole compounds, and water molecules in the electrolyte membrane through the discrete Fourier transformation**, the calculations were consistent with the experimental results, providing a theoretical examination of the phenomenon.

* methyl imidazole: compounds containing atoms other than carbon atoms in the five-membered ring and containing at least one nitrogen atom

* discrete Fourier transform: Fourier transform of discrete input signals, which theoretically calculates chemical actions and bonds

◦ The conduction of hydrogen ions through the phosphoric acid electrolyte occurs through the Grotthuss pathway* where the hydrogen ions jump between phosphoric acid and phosphoric acid. At this time, if a methyl group is present in the azole compound of the polymer electrolyte membrane, the acidic hydrogen is reduced, so the efficiency of the Grotthuss pathway and the hydrogen ion conductivity are lowered, confirming that the hydrogen fuel cell performance further improved due to less water absorption and less phosphoric acid leakage.

* Grotthuss pathway: When excess hydrogen ions or hydrogen ion defects are present in neighboring molecules, the process of diffusing hydrogen ions through the hydrogen bonding network by repeating covalent bond formation and cleavage.

□ Professor Jae-Suk Lee said, "This study drew a direct performance improvement method of high-temperature polymer membrane fuel cells, which are in the spotlight as next-generation building fuel cells, through convergence studies of materials, unit cells, and computational science. In the future, as the supply of fuel cells in homes expands, it is expected to contribute to promoting eco-friendly hydrogen economy by using heating and hot water using waste heat along with distributed power generation."

□ The research was led by Professors Jae-Suk Lee, Chanho Pak, and Joo-Hyoung Lee and led by Dr. Joseph Jang and Ph.D. students Do-Hyung Kim and Byeol Kang with support from the GIST Grubbs Center for Polymers and Catalysis, the Korea Institute of Energy Technology Evaluation and Planning, and the Ministry of Trade, Industry & Energy and was published online on January 3, 2021, in *ACS Applied Materials & Interfaces*, a renowned journal in the field of materials science.

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