NREL Highlights SCIENCE

Computer Modeling Illuminates Degradation Pathways of Cations in Alkaline Membrane Fuel Cells

Cation degradation insights obtained by computational modeling could result in better performance and longer lifetime for alkaline membrane fuel cells.

Scientists at the National Renewable Energy Laboratory (NREL) used density functional theory (DFT) calculations to investigate the degradation pathways of different substituted trimethylammonium cations used in alkaline membrane fuel cells (AMFCs). AMFCs are promising next-generation fuel cell devices that can utilize non-precious catalysts, thereby greatly reducing cost. In AMFCs, an anion exchange membrane (AEM) with cations tethered to the polymer backbone is used to allow hydroxide to transport between the electrodes. However, the stability of cations limits the performance and lifetime of AMFCs.

NREL researchers identified two potential degradation pathways: S_N2 and Hofmann elimination. The energy barriers of Hofmann elimination were found to be lower than the S_N2 pathway, making Hofmann elimination the main pathway by which substituted trimethylammonium cations degrade. Because Hofmann elimination has been found to be the more vulnerable pathway for degradation, in order to improve cation stability, the energy barriers of Hofmann elimination could be increased by introducing steric effects. NREL researchers modeled different steric effects and concluded that several are effective in increasing cation stability. With the help of computational modeling, more cations are being modeled, synthesized, and tested at NREL to further improve their stability in AEM, promising cheaper and more durable AMFCs in the future.

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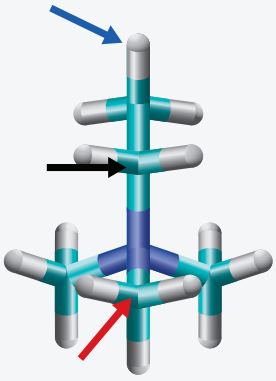
Reference: Long, H.; Kim, K.; Pivovar, B.S. (2012). "Hydroxide Degradation Pathways for Substituted Trimethylammonium Cations: A DFT Study." *J. Phys. Chem. C* 116 (17), 9419–9426.



Ethyltrimethyl ammonium degradation pathway. Blue: Hofmann; Black: ethyl S_N2; Red: methyl S_N2. Illustration by Hai Long, NREL

Key Research Results

Achievement

NREL scientists used computational modeling to investigate cation degradation pathways to improve the lifetime of alkaline membrane fuel cells.

Key Result

Hofmann elimination was found to be the main degradation pathway. Some steric effects are useful to make the cation more stable.

Potential Impact

This research can lead to a more stable anion exchange membrane and thus a less expensive and more durable fuel cell in the future.

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