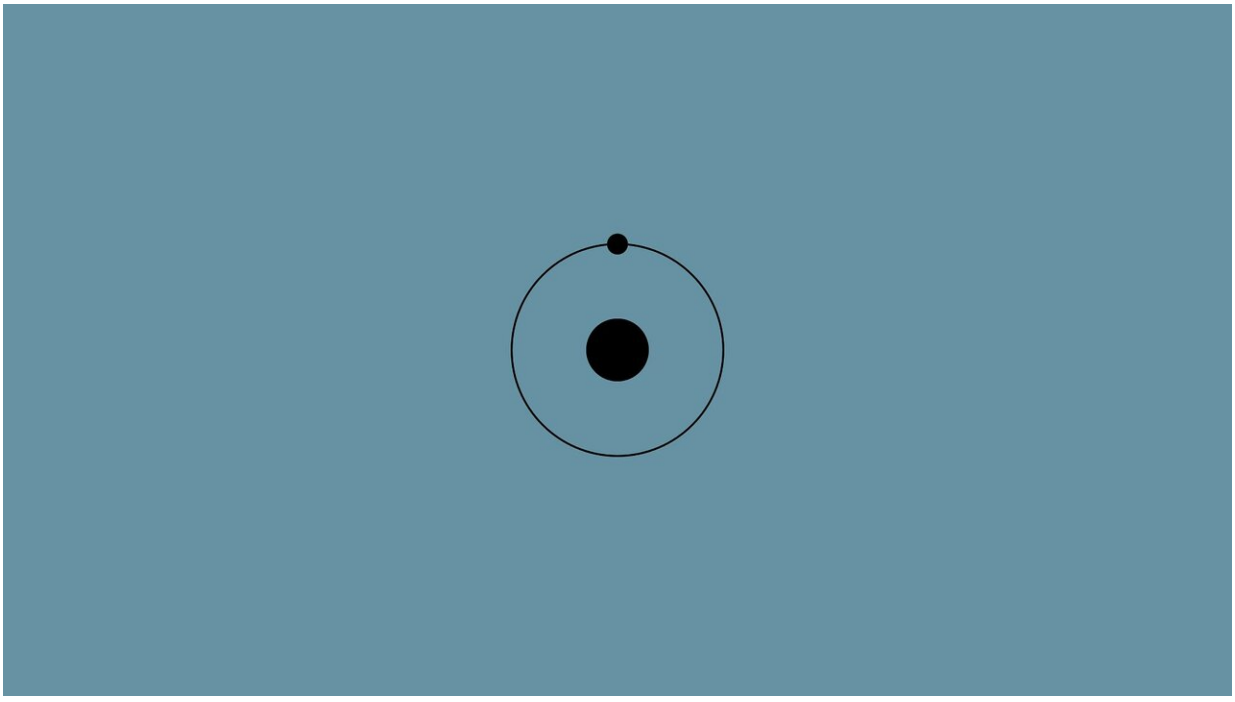
A new fuel cell electrolyte

June 29 2021



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As far back as the 1930s, inventors have commercialized fuel cells as a versatile source of power. Now, researchers from Japan have highlighted the impressive chemistry of an essential component of an upcoming fuel cell technology.

In a study recently published in the *Journal of Physical Chemistry Letters*, researchers from the University of Tsukuba have revealed successive

proton transport—energy transfer—in an advanced carbon-based crystal for future fuel cells, and the chemistry that underpins this phenomenon.

Such crystals are exciting as solid electrolytes—energy transfer media—in upcoming fuel cell technologies. Solid electrolytes have advantages, such as high power efficiency and long-term stability, which some electrolytes lack. Solid electrolytes based on imidazole are common focuses of study. Researchers hypothesize that crystals of imidazolium hydrogen succinate can exhibit successive proton transport, also known as proton jumping. At present, this has not been rigorously confirmed, something the researchers at the University of Tsukuba aimed to address.

"A wide range of lab work and computer simulations are consistent with unidirectional proton transport in crystals of imidazolium hydrogen succinate," says lead and senior author of the study, Professor Yuta Hori. "Because this hypothesis requires further testing, we computed the molecular energy versus molecular geometry of our crystals, and compared our results with experimental data."

To do this, the researchers studied known crystal structures to investigate a chemical structure known as hydrogen bonds. Hydrogen dynamics on these bonds facilitate proton transport within the crystals and can be characterized experimentally by infrared spectroscopy.

"The spectroscopy results were clear," explains Hori. "We found that at 100°C, compared with 30°C, there was a shift to higher energy in a peak that pertains to proton transport."

Furthermore, the researchers' calculated peaks—those corresponding to chemical units that strongly contribute to hydrogen bonding—were consistent with the experimental data.

"We used these results to construct a model that traced how a proton is transferred from one imidazole unit to another," says Hori. "Our calculated potential energy surface provided geometric and energetic data that are consistent with proton jumping."

Fuel cells are used today to power a wide range of civil infrastructure and technologies, and typically produce few emissions. Improving the utility of fuel cells in more diverse applications, achieved in part by understanding how they work, will help minimize wasted power in the coming years.

More information: Yuta Hori et al, Proton Conduction Mechanism for Anhydrous Imidazolium Hydrogen Succinate Based on Local Structures and Molecular Dynamics, *The Journal of Physical Chemistry Letters* (2021). DOI: 10.1021/acs.jpclett.1c01280

Provided by University of Tsukuba