

# Chemists explain the molecular workings of promising fuel cell electrolyte

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Researchers from New York University and the Max Planck Institute in Stuttgart reveal how protons move in phosphoric acid in a *Nature Chemistry* study that sheds new light on the workings of a promising fuel cell electrolyte.

Phosphoric acid fuel cells were the first modern [fuel cell](#) types to be used commercially and have found application as both stationary and automotive power sources. Their high efficiency as combined power and heat generators make them attractive targets for further development. In the cell, phosphoric acid functions as the medium (or "electrolyte") that transports protons produced in the reaction that decomposes the fuel across the cell. Indeed, phosphoric acid has the highest proton conductivity of any known substance, but what makes it work so well as a proton conductor has remained a mystery.

Efficient proton transport across a fuel cell is just one of several technical challenges that must be tackled before this technology can be applied on a massive scale. The key to this problem is the identification of a suitable electrolyte material. Hydrated polymers are often employed, but these must operate at temperatures below the boiling point of [water](#), which limits their utility. Phosphoric acid fuel cells and other phosphate-based cells, by contrast, can be operated at substantially higher temperatures.

Chemists have sought a molecular level understanding of proton conduction phenomena for more than 200 years. The earliest studies

concerned water and can be traced back to a landmark paper in 1806 by the German chemist Theodor von Grotthuss. In this paper, Grotthuss suggested that excess protons in aqueous acids are not themselves transported, but rather it is the chemical bonding pattern they create that is transported via a series of short hops of protons between neighboring [water molecules](#). Such hops occur through the [hydrogen bonds](#) that connect water molecules into a network.

One can liken this process to an old-time fire brigade in which each fireman in a long line holds a bucket of water in his left hand. A fireman at the end of the line receives a new water bucket in his right hand, so in order to make the transport of water down the line as efficient as possible, he passes the bucket in his left hand to the right hand of his neighbor. The neighbor, who now holds buckets in his left and right hands, passes the bucket in his left hand to the right hand of the next fireman in the line, and the process continues like this until the person at the opposite end of the line holds two buckets. Overall, water is transported down the line, but it is not the same bucket being passed in each transfer.

Of course, the transport of excess protons in water is not this simple—it involves complex rearrangements of the hydrogen bonds at each transfer step to accommodate the diffusing chemical bonding pattern. Because of this, proton transport in water appears to be a step-wise process. Water faces other limitations—it cannot function as an intrinsic proton conductor but must have protons added to it to create aqueous acid solutions before any noticeable proton transport occurs.

The *Nature Chemistry* study contrasted proton conduction in phosphoric acid with excess protons in aqueous solutions. In their work, the researchers carried out a type of "computerized experiment" or "simulation" in which no prior knowledge of the chemical processes is required. The only input is the atomic composition of phosphoric acid

(hydrogen, oxygen, and phosphorus). Based on this input, the atoms' motion in time is determined from the fundamental laws of physics. In this way, the proton conduction mechanism can be allowed to unfold and be discovered directly from the simulation output.

Their results showed that proton motion in phosphoric acid is a highly cooperative process that can involve as many as five phosphoric acid molecules at a time serving as a kind of temporary "proton wire" or chain. The basic findings are:

- In contrast to the step-wise mechanism that operates in water, phosphoric acid transfers protons in a more "streamlined" fashion, in which protons move in a concerted manner along one of these temporary wires.
- Eventually, it becomes energetically unfavourable for this wire to sustain this proton motion. Hence, the system then seeks to resolve this unfavourable condition by breaking one of the hydrogen bonds in this temporary wire and forming a new wire arrangement with other nearby phosphoric acid molecules. New wire arrangements persist until they can no longer sustain the proton motion in them, at which point they break and new wires are formed. This process of forming and breaking the short wires allows for a steady proton current and overall high proton conductivity.

Although phosphoric acid has its advantages in fuel cell applications, phosphoric acid fuel cells still are not as powerful as other types of cells and, as pure power sources, are not as efficient. However, an understanding of the basic proton transport mechanism can help improve the design of such cells or suggest other phosphate based materials that could serve as the proton carrier.

Provided by New York University

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