Renewable energy technology news

A key chemical reaction -- in which the movement of protons between the surface of an electrode and an electrolyte drives an electric current -- is a critical step in many energy technologies, including fuel cells and the electrolyzers used to produce hydrogen gas.

For the first time, MIT chemists have mapped out in detail how these proton-coupled electron transfers happen at an electrode surface. Their results could help researchers design more efficient fuel cells, batteries, or other energy technologies.

"Our advance in this paper was studying and understanding the nature of how these electrons and protons couple at a surface site, which is relevant for catalytic reactions that are important in the context of energy conversion devices or catalytic reactions," says Yogesh Surendranath, a professor of chemistry and chemical engineering at MIT and the senior author of the study.

Among their findings, the researchers were able to trace exactly how changes in the pH of the electrolyte solution surrounding an electrode affect the rate of proton motion and electron flow within the electrode.

MIT graduate student Noah Lewis is the lead author of the paper, which appears today in Nature Chemistry. Ryan Bisbey, a former MIT postdoc; Karl Westendorff, an MIT graduate student; and Alexander Soudackov, a research scientist at Yale University, are also authors of the paper.

Proton-coupled electron transfer occurs when a molecule, often water or an acid, transfers a proton to another molecule or to an electrode surface, which stimulates the proton acceptor to also take up an electron. This kind of reaction has been harnessed for many energy applications.

"These proton-coupled electron transfer reactions are ubiquitous. They are often key steps in catalytic mechanisms, and are particularly important for energy conversion processes such as hydrogen generation or fuel cell catalysis," Surendranath says.

In a hydrogen-generating electrolyzer, this approach is used to remove protons from water and add electrons to the protons to form hydrogen gas. In a fuel cell, electricity is generated when protons and electrons are removed from hydrogen gas and added to oxygen to form water.

To overcome that obstacle, the MIT team developed a way to design electrode surfaces that gives them much more precise control over the composition of the electrode surface. Their electrodes consist of sheets of graphene with organic, ring-containing compounds attached to the surface. At the end of each of these organic molecules is a negatively charged oxygen ion that can accept protons from the surrounding solution, which causes an electron to flow from the circuit into the graphitic surface.

"We can create an electrode that doesn"t consist of a wide diversity of sites but is a uniform array of a single type of very well-defined sites that can each bind a proton with the same affinity," Surendranath says. "Since we have these very well-defined sites, what this allowed us to do was really unravel the kinetics of these processes."

Using this system, the researchers were able to measure the flow of electrical current to the electrodes, which allowed them to calculate the rate of proton transfer to the oxygen ion at the surface at equilibrium -- the state when the rates of proton donation to the surface and proton transfer back to solution from the surface are equal. They found that the pH of the surrounding solution has a significant effect on this rate: The highest rates occurred at the extreme ends of the pH scale -- pH 0, the most acidic, and pH 14, the most basic.