Proton pinball on the catalyst

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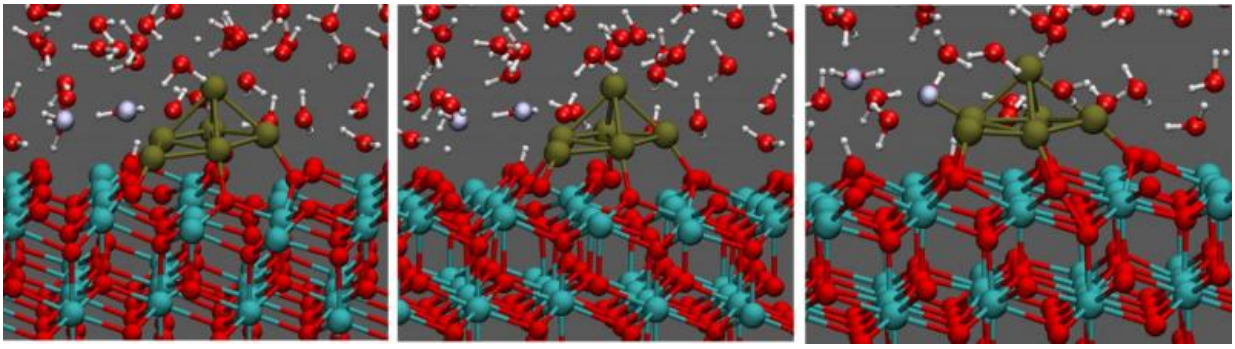

Water on catalyst. Credit: SISSA/CNR IOM

Thanks to a reaction that resembles a sort of proton pinball game, a thin layer of moisture on the surface of a catalysts can improve the efficiency of fuel cells, devices used to transform chemical energy (a fuel like hydrogen, for example) directly into electricity without releasing greenhouse gases in emissions. The study was coordinated by IOM CNR/ SISSA.

The function of fuel cells is to transform chemical energy into electricity through a chemical reaction. When this technology is mature enough it will be possible to use a fuel like hydrogen without emitting CO2 into the atmosphere. In the fuel cell, the chemical reaction is facilitated by a catalyst, typically platinum nanoparticles dispersed onto the surface of a durable and reactive material, such as cerium oxide, for example. Before this study, the active areas of these catalysts had been studied under ideal

conditions, at very low temperatures and pressures, removing any dirt and moisture which could be found in the devices under ordinary working conditions. Stefano Fabris, a Physicist at the International School for Advanced Studies (SISSA) of Trieste and CNR-IOM Istituto Officina dei Materiali, and colleagues, however, wanted to study a system in realistic conditions, in this case adding a thin layer of water onto the catalyst. The team made some interesting discoveries: it seems the moisture, rather than making the processes less efficient, gives atoms in transit a "boost" thus significantly improving the overall efficiency of the system. The study, coordinated by Fabris, was published in the *Journal of the American Chemical Society*.

Fabris and colleagues' work is based on computer simulations. "This is a not an insignificant aspect, because traditional experimental techniques do not allow us to obtain detailed information about what happens at the interface between the surface of the catalyst and a liquid such as water. In this way, the atomic layers that separate the solid and the water remain a largely unexplored world, as difficult to measure as the core of a planet," explains Fabris. "The pressure and temperature conditions prevent a direct view at the experimental level. We must therefore find other ways to investigate this kind of phenomena, such as using these numerical simulations."

Chain Reaction

Fabris and colleagues reconstructed the physical system in detail, exactly where the surface of the catalyst comes into contact with one or more layers of water molecules and observed its evolution in real time. "First, we noticed that the water in contact with the catalyst breaks down, in part, into hydrogen ions, or protons, and hydroxide ions (OH-).

This was not completely unexpected, says Matteo Farnesi Camellone, CNR-IOM (Istituto Officina dei Materiali) Researcher and first author

of the work, adding that an effect like this could have been imagined a priori. "The really interesting part happens after this breakdown," says Farnesi Camellone. When there is a certain number of protons and hydroxide ions on the surface, a so-called proton chain occurs: "a sort of pinball game where the OH- groups pass a free proton back and forth incessantly, binding it and releasing it. In the process water molecules form and break up continuously, while the protons continue to bounce and travel long distances along the surface." The consequences for the catalytic process are positive. "All of this movement helps transport molecules between the active zones of the material. We measured increases in transport and release speed several times, the efficiency of the catalyst actually improves."

"This is the first time the catalyst has been studied with water present. Our study, besides showing that the process is favored by moisture, goes beyond to explain what happens in the material in detail, which is important knowledge for designing better fuel cells," says Fabris.

More information: Matteo Farnesi Camellone et al. Catalytic Proton Dynamics at the Water/Solid Interface of Ceria-Supported Pt Clusters, *Journal of the American Chemical Society* (2016). DOI: 10.1021/jacs.6b03446

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