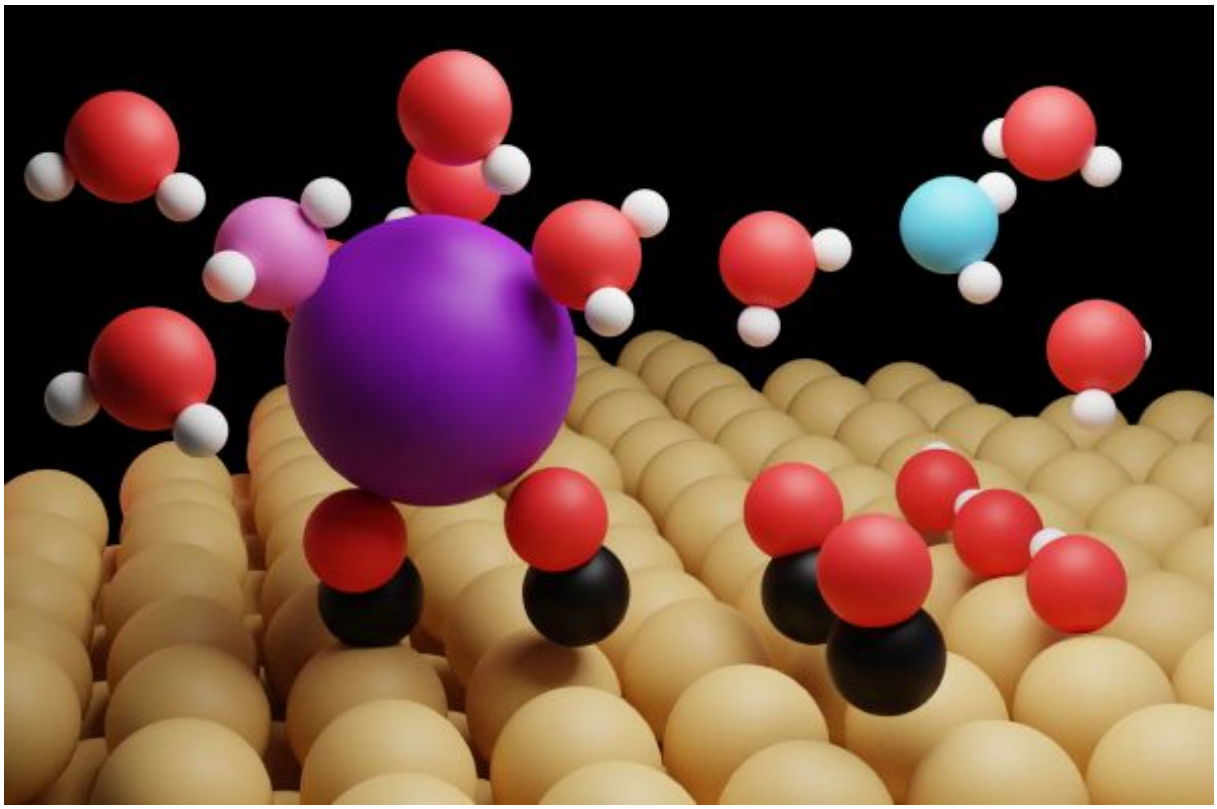

Water is not just a liquid: The right water arrangement favors CO2 conversion into useful chemicals

Water is a key ingredient in technologies to make sustainable fuels such as CO2 electrolysis, but so far was viewed just as a passive element. ICFO and ICIQ researchers have now shown in a Nature Catalysis study that interfacial water plays an active role in CO2 reduction, as it regulates the access of CO2 to the reactive interface for the subsequent production of multicarbon chemicals.

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As part of the effort to mitigate global warming, scientists are exploring sustainable ways to reduce greenhouse gases. One of the strategy to do so is **CO2 electroreduction (CO2R)**, a process that uses electricity to convert captured CO2 into widely used multicarbon chemicals that are today produced from fossil fuels, such as **ethylene** and **ethanol**.
In CO2R, CO2 molecules adsorb on a cathode catalyst and break and recombine into higher

energy molecules feeding from electrons and protons from water. In this picture, water has been commonly seen as a passive element, but things change when reaction speed increases. ICFO researchers, **Dr. Anku Guha**, **Dr. Barbara Polesso**, **Prathama Haldar**, **Ranit Ram**, **Adrian Pinilla-Sanchez**, **Dr. Indrajit Mondal**, and **David Kernan**, led by **Prof. at ICFO F. Pelayo Garcia de Arquer**, together with researchers at ICIQ led by Nuria Lopez, have take one step further by investigating the role of interfacial water in CO2R. Implementing for the first time operando Raman spectroscopy in a high-performance industrially relevant reactor, the team has been able to see that **water** is not a passive element but **regulates CO2 access to the catalyst interface and ensuing reaction steps**.

Water can be classified depending on the way it is structured through hydrogen bonds. Water molecules over a polarized surface can form ordered or disordered networks, and can also be aligned or misaligned with the electric field at the interface. According to the study, published in Nature Catalysis, **a certain water arrangement (disordered water aligned with the electric field) promotes the conversion of CO2** into valuable chemicals. In contrast, other configurations where water is increasingly ordered supress the desired reaction. i¿½We we e surprised to find that water itself could act as a gatekeeper for CO2i¿½ says Dr. Anku Guh , first author of the article. i¿½But we saw that its structure at the interface can deter ine whether CO2 can access the catalyst and undergo the desired reaction.i¿ ? These insights were made possible by performing **Raman spectroscopy during operation at industrially relevant current densities**, which the researchers achieved for the first time. Previous studies relied on in-situ Raman spectroscopy, which probes the catalyst in its reaction environment but typically under simplified conditions far from practical settings. As a result, the active involvement of interfacial water in CO2R remained beyond the reach of this conventional approach, a limitation the new technique finally overcomes.

The plan now, the authors say, is to tune the cathode environment by adjusting parameters such as the catalyst's coating or the external temperature, so that the right kind of water network is promoted and maintained at the interface. Prof. Pelayo Garcia de Arquer, lead researcher of the study, remarks that i¿½further understanding and actively controlling wat r could be a turning point in the future development of CO2 conversion technologies.i¿

Reference:

Guha, A., Seemakurthi, R.R., Polesso, B. et al. Operando resolution of CO2 electrolysis interfaces at application-relevant current density reveals water gating. Nat Catal (2026). https://doi.org/10.1038/s41929-026-01620-w

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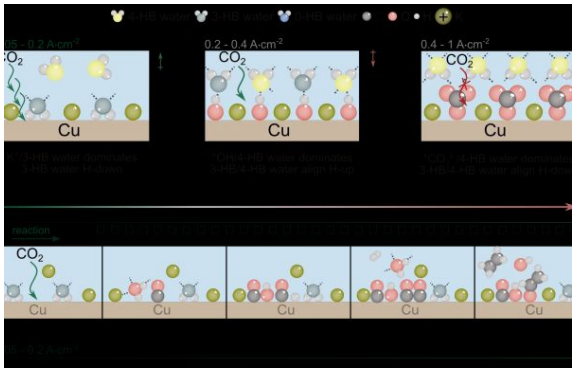

Schematic of the CO2 reduction and the role of interfacial water. Interfacial water progressively reorganizes with increasing current density. Source: Nature Catalysis.