Trinity's research on how water dissociates on cobalt oxide nanoislands published in Nature Communications.

Ussher Assistant Professor Max García-Melchor and his co-workers from Aarhus University and Stanford University, have shed light into the water dissociation process on cobalt oxide nanoislands, which show great promise as Earth-abundant catalysts to produce H_2 as fuel and develop sustainable energy technologies.

For the first time, atom-resolved scanning tunnelling microscopy (STM), X-ray photoelectron spectroscopy (XPS), and computational modelling have demonstrated that water dissociates at the under coordinated metal edge sites of the cobalt nanoislands. Surprisingly, the authors find that an additional water molecule acts to promote all the elementary steps of the dissociation process and subsequent hydrogen migration, thus revealing the important assisting role of water molecules in its own dissociation on a metal oxide. Inspired by these findings, the authors also use computational methods to evaluate the performance of these cobalt nanoislands towards the electrochemical water oxidation reaction. Theoretical simulations indicate that the nanoparticle metal edges of a O-Co-O trilayer supported on a Au(111) surface display very favourable energetics for this process, predicting an overpotential of only 330 mV.

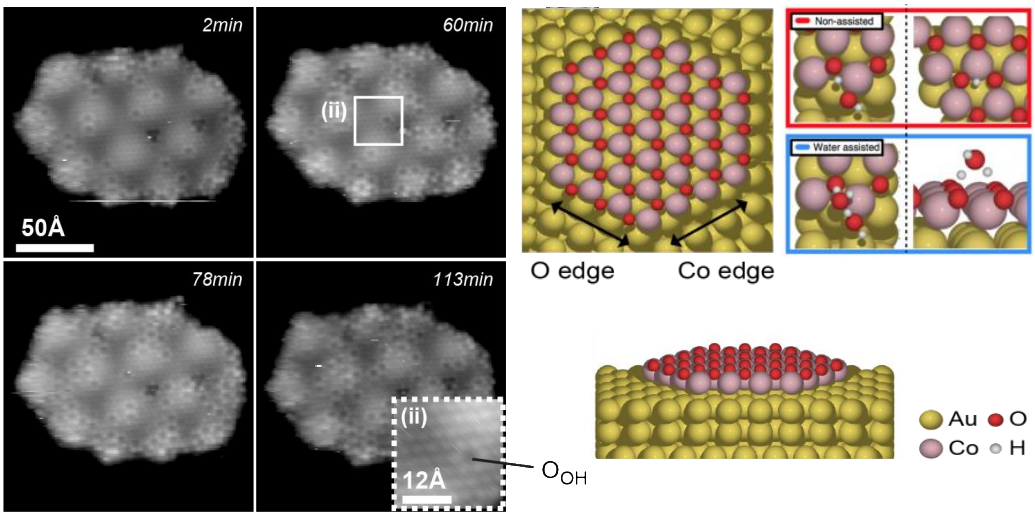

Figure: Images from an STM movie recorded in water vapour environment (left) and structure models of cobalt oxide nanoislands employed in theoretical simulations (right).

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