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Surface Proton Hopping and Coupling Pathway of Water Oxidation on Cobalt Oxide Catalyst. HIEU PHAM, Lawrence Berkeley National Laboratory, MU-JENG CHENG, University of California, Berkeley, HEINZ FREI, LIN-WANG WANG, Lawrence Berkeley National Laboratory — We propose an oxidation pathway of water splitting on cobalt oxide surface with clear thermodynamic and kinetic details. The density-functional theory studies suggest that the coupled proton-electron transfer is not necessarily sequential and implicit in every elementary step of this mechanistic cycle. Instead, the initial O-O bond could be formed by the landing of water molecule on the surface oxos, which is then followed by the dispatch of protons through the hopping manner and subsequent release of di-oxygen. Our theoretical investigations of intermediates and transition states indicate that all chemical conversions in this pathway, including the proton transfers, are possible with low activation barriers, in addition to their favorable thermodynamics. Our hypothesis is supported by recent experimental observations of surface superoxide that is stabilized by hydrogen bonding to adjacent hydroxyl group, as an intermediate on fast-kinetics catalytic site.

Hieu Pham
Lawrence Berkeley National Laboratory

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