Selective Electrochemical Generation of Hydrogen Peroxide from Water Oxidation

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Water is a life-giving source, fundamental to human existence, yet over a billion people lack access to clean drinking water. The present techniques for water treatment such as piped, treated water rely on time and resource intensive centralized solutions. In this work, we propose a decentralized device concept that can utilize sunlight to split water into hydrogen and hydrogen peroxide. The hydrogen peroxide can oxidize organics while the hydrogen bubbles out. In enabling this device, we require an electrocatalyst that can oxidize water while suppressing the thermodynamically favored oxygen evolution and form hydrogen peroxide. Using density functional theory calculations, we show that the free energy of adsorbed OH* can be used to determine selectivity trends between the 2e(-) water oxidation to H2O2 and the 4e(-) oxidation to O2. We show that materials which bind oxygen intermediates sufficiently weakly, such as SnO2, can activate hydrogen peroxide evolution. We present a rational design principle for the selectivity in electrochemical water oxidation and identify new material candidates that could perform H2O2 evolution selectively.

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