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Designing multifunctional Metal Telluride based Electrocatalysts for Sea Water Electrolysis and Oxygen Reduction

Abstract: The relentless overconsumption of fossil fuels has led to their rapid depletion, triggering a growing energy crisis and numerous environmental concerns. Developing energy conversion systems to produce green energy from renewable resources as an alternative to fossil fuels is crucial for creating a sustainable energy future. Among various clean energy alternatives, hydrogen stands out as a highly promising solution, with water electrolysis being one of the most promising technologies for producing green hydrogen. This process relies on two key half-reactions: the oxygen evolution reaction (OER) at the anode and the hydrogen evolution reaction (HER) at the cathode. However, the oxygen evolution reaction is the most crucial step for efficient water splitting. With freshwater resources being limited and increasingly strained by traditional electrolysis methods, seawater, a vast and readily available resource, presents an appealing alternative. Seawater electrolysis enables the direct use of saline water to produce hydrogen fuel, offering a green, renewable energy source without competing for potable water reserves. However, seawater electrolysis possesses a challenge of suppressing chlorine evolution reaction (CER) in an alkaline environment, which leads to the undesirable formation of chlorine gas (Cl_2), thus affecting the oxygen evolution reaction (OER). We investigated the electrocatalytic activity of transition metal telluride-based electrocatalysts in oxygen evolution reaction and hydrogen evolution reaction through seawater electrolysis. One of the key findings of this research is that these telluride surfaces favor OER over CER thereby, removing the surface passivation and poisoning by the high salinity of naturally occurring seawater. Furthermore, we explore the efficacy of our catalyst for oxygen reduction reaction in an alkaline seawater medium. A key focus of our research was assessing the catalyst's ability to suppress the CER in seawater electrolysis, thereby minimizing chlorine gas formation and enhancing OER efficiency. To further elucidate the structure–property relationships governing catalytic activity, we integrated our experimental findings with theoretical insights through density functional theory (DFT) analysis.