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BEYOND ULTRAVIOLET: OXYGEN-VACANT ZrO_{2-x} FOR VISIBLE-IR-LIGHT-DRIVEN WATER SPLITTING

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Solar energy conversion through photocatalysis offers a promising solution for the rising global demand for clean and sustainable energy. Low-cost, efficient photocatalysts for water splitting have emerged as a viable path for clean hydrogen production, driven by significant advancements in recent decades. Reduced transition metal oxides with oxygen vacancies (OV) have proven to be candidates for studying the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) in photocatalytic water splitting. Their photocatalytic ability originates from the ideal properties of a narrow band gap and the existence of favourable trap states within the forbidden band due to the presence of OVs, which can facilitate the adsorption and activation of water molecules, promoting the HER. In this work, photocatalytic hydrogen production of highly reduced and oxygen-deficient $ZrO_{2-x}$was investigated under visible and IR light. The ZrO_{2-x} catalyst was synthesized by treating the ZrO_2 with $NaBH_4$ and annealing at 550 ^oC and 850 ^oC in a nitrogen atmosphere. Hydrogen evolution rates of 28.98 µmol g^{-1} h^{-1} and 3.50 µmol g^{-1} h^{-1} under Vis-IR illumination at an intensity of 100 mW cm^{-2} were noted for the 850 ^oC and 550 ^oC heated ZrO_{2-x} catalysts, respectively. Scanning electron microscopy analysis revealed micro-sized catalyst particles. Energy-dispersive X-ray spectroscopy confirmed the successful incorporation of Boron dopants within the ZrO_2 lattice. The concentration of dopants and the concentration of OVs have increased in the 850 ^oC catalyst compared to the 550 ^oC catalyst. The presence of these dopants and OVs is expected to promote the formation of small polarons, potentially leading to improved light absorption and charge separation. The current results warrant further studies on the photocatalytic activity of reduced ZrO_2.

Keywords: Hydrogen evolution rates (HER), Oxygen-vacancies, Photocatalysts, Reduced-compounds, ZrO_2