

**Title: The efficacy of rare-earth doped V<sub>2</sub>O<sub>5</sub> photocatalyst for removal of pollutants from industrial wastewater**

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**Abstract:** [Photocatalysis](#) is regarded as one of the most environmentally benign methods of mitigating the effects of textile wastewater. Despite the fact that various semiconducting [metal oxides](#) are used in photocatalysis, their performance is still insufficient. In this study, the [hydrothermal method](#) was used to synthesize rare-earth (RE) elements [Holmium (Ho) and [Ytterbium](#) (Yb)] doped vanadium pentoxide (V<sub>2</sub>O<sub>5</sub>) to improve its photocatalytic efficiency. The effect of RE ions on the photocatalytic efficiency of doped V<sub>2</sub>O<sub>5</sub> has also been analyzed from both the experimental and first-principle [density functional theory](#) (DFT) methods. The stable orthorhombic crystal structure of doped V<sub>2</sub>O<sub>5</sub> is confirmed by the X-ray diffraction with no secondary phase, and high-stressed conditions are generated for the 3 mol.%. The [crystallite](#) size, strain, and dislocation density are calculated to perceive the doping effect on the bare V<sub>2</sub>O<sub>5</sub>. The optical characteristics have been measured using UV–vis spectroscopy. The absorptions are found to be increased with increasing doping concentrations; however, the bandgap remains in the visible range. The photocatalytic properties are examined for the bare compound with varying pH, with the highest efficiency exhibited for pH 7. Moreover, it is observed that the RE ions significantly impact the catalytic behavior of V<sub>2</sub>O<sub>5</sub>. The degradation efficiency is improved by 93 % and 95 % for the 3 mol.% of Ho and Yb-doped V<sub>2</sub>O<sub>5</sub> samples within 2 h, respectively, and the mechanism behind these extraordinary efficiencies has been explained thoroughly.

**Keywords:** Rare-earth doped V<sub>2</sub>O<sub>5</sub> Photocatalytic degradation Hydrothermal synthesis Density Functional Theory (DFT) Crystal structure and defects

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