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Passivated Co-doping Approach to Bandgap Narrowing of Titanium Dioxide with Enhanced Photocatalytic Activity

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GRAPHICAL ABSTRACT

Highlights

- TiO_2 doped with (V_{Ti}-N_O) co-dopant is proposed to achieve an enhanced vis-photocatalytic activity of TiO_2.
- The relationship between the redox potentials of <remove-image> and <remove-image> and the band edges position of various passivated co-dopants in TiO_2 is obtained from the results of first-principles electronic structure calculations.
- (V_{Ti}-N_O) co-doping of TiO_2 satisfies the requirement of a reduced bandgap optimized for the visible light absorption without creating recombination centers.
- <<Propose a requirement for enhancing visible light absorption while keep high production of <remove-image> and <remove-image>.>>

Abstract

Aiming for the enhanced photocatalytic activity of titanium dioxide (TiO_2), we probe various co-doping pairs of impurity atoms in TiO_2 in search of the right co-dopants which can reduce the bandgap without creating recombination centers. To confirm the band edges and the relative positions of impurity levels, we perform first-principles density-functional-theory calculations within the local density approximation as well as the hybrid functional approach. From the analysis of the bandgaps of doped-TiO_2 and the defect levels, we propose that the vanadium-nitrogen (V-N) pair is a suitable passivated co-dopant in TiO_2. By doping TiO_2 with the V-N pair, the bandgap of TiO_2 is reduced; enhancing the