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DFT studies of photocatalytic properties of barium titanate doped with vanadium and tungsten for hydrogen production via water splitting.

Experimental studies have demonstrated that pure BaTiO3 can serve as a catalyst for hydrogen production via water splitting. However, its large energy band gap prevents activation under visible light. This study explores the potential of using visible light, the most abundant component of solar energy, to drive water splitting by modifying BaTiO3's electronic and optical properties through Mono-doping and Co-doping. Using first-principles density functional theory (DFT) calculations, the effects of vanadium and tungsten (W) as dopant were analyzed. Doping lowered the energy required for electronic transitions in BaTiO3. Further confirmation of impurity states generated by doping was provided by calculating the DOS and values of charge density difference. In terms of the optical properties, the doped models exhibited widening of absorption edges in comparison to pure BaTiO3, resulting in absorption peaks extending into the visible light region, thereby effectively improving the overall optical performance

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