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Tailoring the photocatalytic properties of anatase TiO_2 by B - TM (TM = Pt, Ta, V) co-doping

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In the present work, the electronic and optical properties of (B, TM) co-doped (TM = Pt, Ta, V) anatase TiO_2 were investigated using modified density functional theory (DFT) calculations, in order to provide insight into the synergistic effect of co-doping with various elements on the photoactivity of TiO_2. We considered two combinations for each co-doped sample, with TM atom replacing Ti atom and B atom either replacing O atom or embedding interstitially into TiO_2 lattice. The calculations showed that for all studied transition metals, the co-doping is more favorable in the case of interstitially doped boron than for the substitutional one and under the O-rich conditions. For the co-doped systems with B atom substitutionally replacing O atom, a small reduction of the band gap is observed in all the investigated cases. In contrast, the results obtained for the co-doped systems with boron embedded interstitially into TiO_2 lattice, exhibited no band gap narrowing. However, in these systems, the doping induced localized states within the band gap, which could enhance visible light absorption through a two step optical transition from the valence to conduction band.

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