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Understanding the synergistic effects, optical and electronic properties of ternary Fe/C/S-doped TiO2 anatase within the DFT 1 U approach

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ABSTRACT:

Although TiO_2 is an efficient photocatalyst, its large band gap limits its photocatalytic activity only to the ultraviolet region. An experimentally synthesized ternary Fe/C/S-doped TiO_2 anatase showed improved visible light photocatalytic activity. However, a theoretical study of the underlying mechanism of the enhanced photocatalytic activity and the interaction of ternary Fe/C/S-doped TiO_2 has not yet been investigated. In this study, the defect formation energy, electronic structure and optical property of TiO_2doped with Fe, C, and S are investigated in detail using the density functional theory + *U* method. The calculated band gap (3.21 eV) of TiO_2anatase agree well with the experimental band gap (3.20 eV). The defect formation energy shows that the co- and ternary-doped systems are thermodynamically favorable under oxygen-rich condition. Compared to the undoped TiO_2, the absorption edge of the mono-, co-, and ternary-doped TiO_2 is significantly enhanced in the visible light region. We have shown that ternary doping with C, S, and Fe induces a clean band structure without any impurity states. Moreover, the ternary Fe/C/S-doped TiO_2 exhibit an enhanced photocatalytic activity, a smaller band gap and negative formation energy compared to the mono- and co-doped systems. Moreover, the band edges of Fe/C/S-doped TiO_2 align well with the redox potentials of water, which shows that the ternary Fe/C/S-doped TiO_2 is promising photocatalysts to split water into hydrogen and oxygen. These findings rationalize the available experimental results and can assist the design of TiO_2-based photocatalyst materials.