Absorption spectra of trapped holes in anatase TiO$_2$

Charge transport to surface reactive sites is a crucial step in any photocatalytic process. In the most popular photocatalyst - the anatase TiO$_2$, this step is complicated by the fact that photogenerated carriers can trap. Studies of charge trapping and transfer in anatase often employ transient absorption spectroscopy (TAS), but the understanding of the optical absorption due to trapped carriers in TiO$_2$ is incomplete. On the basis of the generalized Δ self-consistent field density functional theory (Δ-SCF DFT) calculations, we attribute the experimentally observed absorption band at 430-550 nm to the interpolaron transitions of the stable surface and subsurface O$^-$ centers and associate the blue shift of the spectra after the photoexcitation with holes migration to surfaces. We also suggest that subsurface hole trapping may contribute to generally lower photocatalytic performance of the anatase (101) surface compared to the (001) surface.

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