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A particular mechanism of the effect of lone pair E Te^{IV} dopant atoms on visible-light photocatalytic activity of anatase TiO_2

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Routine X-Ray Diffraction (XRD) measurements were performed on a powder sample ARL X'TRA Thermo Scientific diffractometer using Cu Kα radiation (wavelength λ = 1.5418 Å). All the studied catalysts were found to be single-phase anatase type (space group $I4_1/amd$) polycrystalline materials. An XRD pattern of the catalyst 0.25 at% Te^{IV}/TiO_2 obtained by annealing under argon atmosphere the co-precipitated hydroxide precursor is shown in Figure S1.

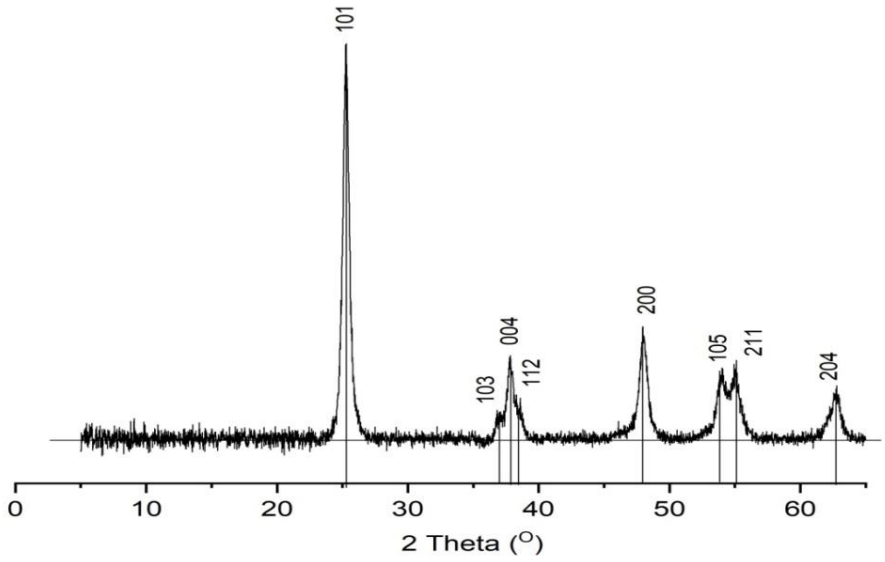

Figure S1 XRD pattern of the catalyst 0.25 at% Te^{IV}/TiO_2 synthesized by annealing the hydroxide precursor under argon atmosphere for 2 h at 500 °C.

Their specific surface area S_{BET} determined by the BET method was found to be ca 58 $m^2\ g^{-1}$ and virtually not dependent on tellurium dopant concentration.

X-ray photoelectron spectroscopy (XPS) measurements were carried out with a Kratos Axis Ultra DLD spectrometer (Kratos Analytcal Ltd, UK) using monochromatic Al Kα radiation ($h\nu$ = 1486.6 eV) and charge compensation. Powder samples were analyzed in the as-prepared state. Atomic concentrations ratios [tellurium] to [titanium] were determined using areas of the Te $3d_{5/2}$ (E_b = 574 eV range) and Ti $2p_{3/2}$ (459 eV range) peaks with Scofield correction and Shirley background subtraction (Figure S2).

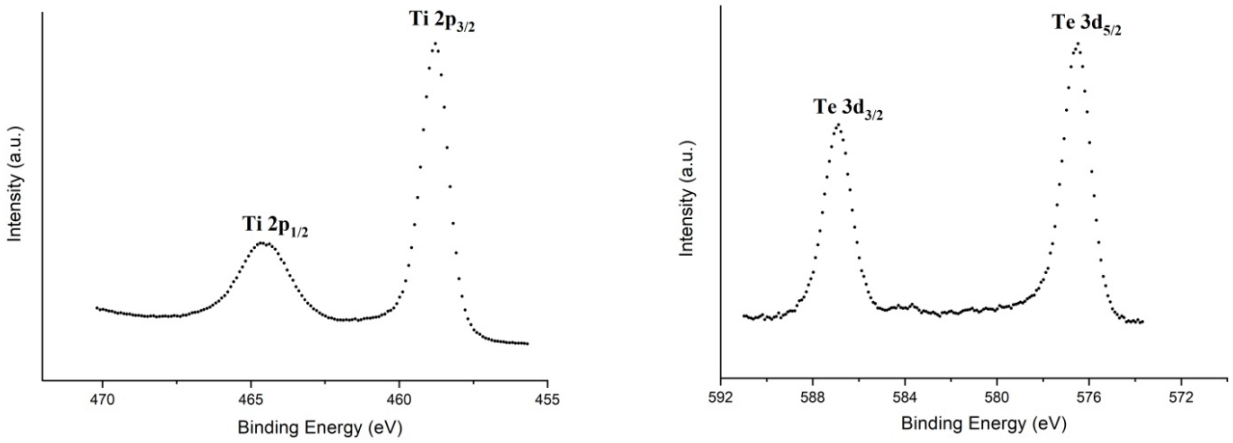

Figure S2 XPS characterization of the tellurium to titanium ratio within nearly 5 nm thin surface adjacent layers of crystallites in the catalyst 0.25 at% Te^{IV}/TiO_2.