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Individual effect of charge balance defects on the photocatalytic activity of Cr^{3+}-modified TiO_2

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Routine X-Ray Diffraction measurements were performed on a powder sample ARL X'TRA Thermo Scientific diffractometer using Cu K_α radiation (wavelength λ = 1.5418 Å).

X-ray photoelectron spectroscopy (XPS) measurements were carried out with a *K*-Alpha X-ray photoelectron spectrometer (ThermoFisher Scientific Inc) using monochromic Al K_α radiation ($h\nu$ = 1486.6 eV) with charge compensation, spot size: 200 μm. Powder samples, to be analyzed in the as-prepared state, were pressed onto indium foil. To analyze high resolution spectra (recorded at pass energy E_p = 40 eV) were fitted using the AVANTAGE software provided by THERMOFISHER SCIENTIFIC INC. To quantify the contribution of the Cr(VI) spectral component (E_b = 579.6 eV) the composite Cr2$p_{3/2}$ XPS peak in the energy region from 572 to 582 eV was analyzed. To take into account the contribution of Ti2*s* satellite peaks, occurring in the same energy region, XP-spectrum of the reference dopant -free TiO_2 sample was used.

^{121}Sb Mössbauer spectra were recorded on a MS-1104 spectrometer and were analyzed by a least-square fitting program. To perform resonant absorption measurements, the 8.5 keV escape peak, produced by Mössbauer gamma rays (E_γ = 37.15 keV) in a thin NaI(Tl) scintillator, was used. During the measurements both $Ca^{121}SnO_3$ source and studied powder sample (absorber) were introduced into the hole of a copper bar immersed in a Dewar flask filled with liquid nitrogen. Under these conditions, the temperature of absorber was close to 100 K and thus allowed to consider the spectral contributions of the eventually present chemically different species of antimony as an acceptable estimate of their abundances.