

Monitoring N719-dye Configurations on (1x n)-Reconstructed Anatase (100) by means of STM: Reversible Configurational Changes upon illumination

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Supplementary Information

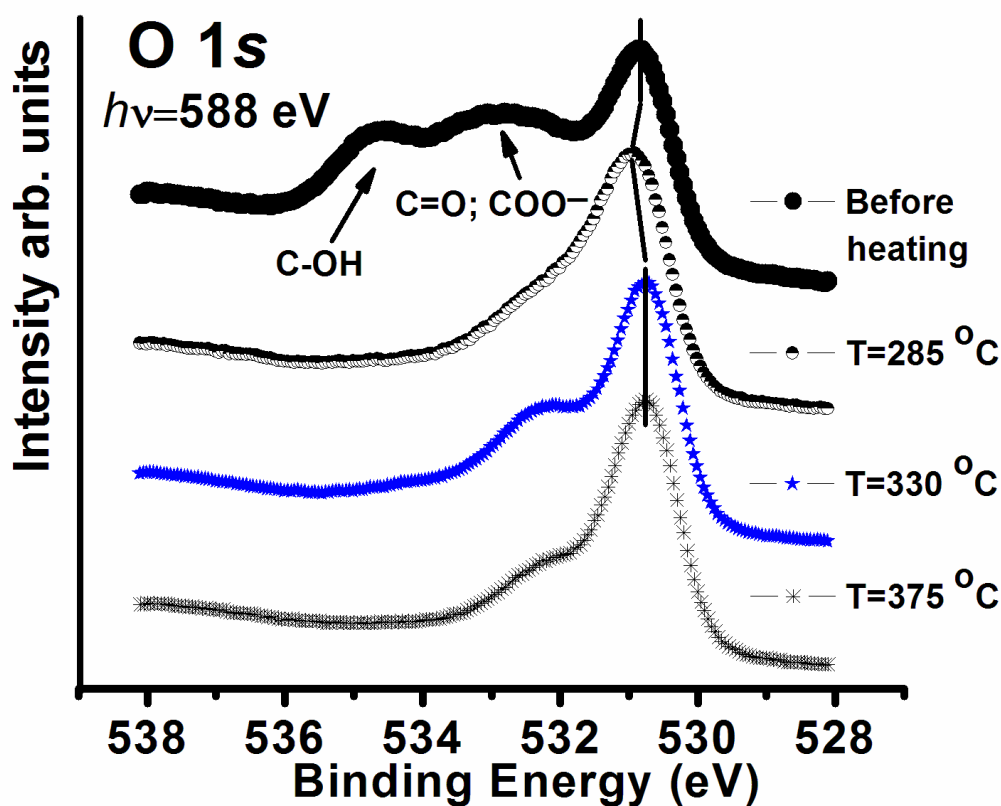


Fig. S1 O 1s photoelectron data. The spectra were normalized against the main peak signal.

As observed, the peaks associated with COO⁻ at 532.8 eV and C-OH at 534.6 eV, decrease in intensity relative to the main peak after the heating. The main peak is associated with the oxygen in the TiO₂, and its intensity increases after heating. The relation between the intensity of the main peak after and before heating is around 1.7 for T= 285 °C and T=330 °C, and approximately 2.0 for T=375 °C. This peak is shifted 0.13 eV to higher binding energy for T=285 °C, but shifts to lower binding energy at higher annealing temperature.

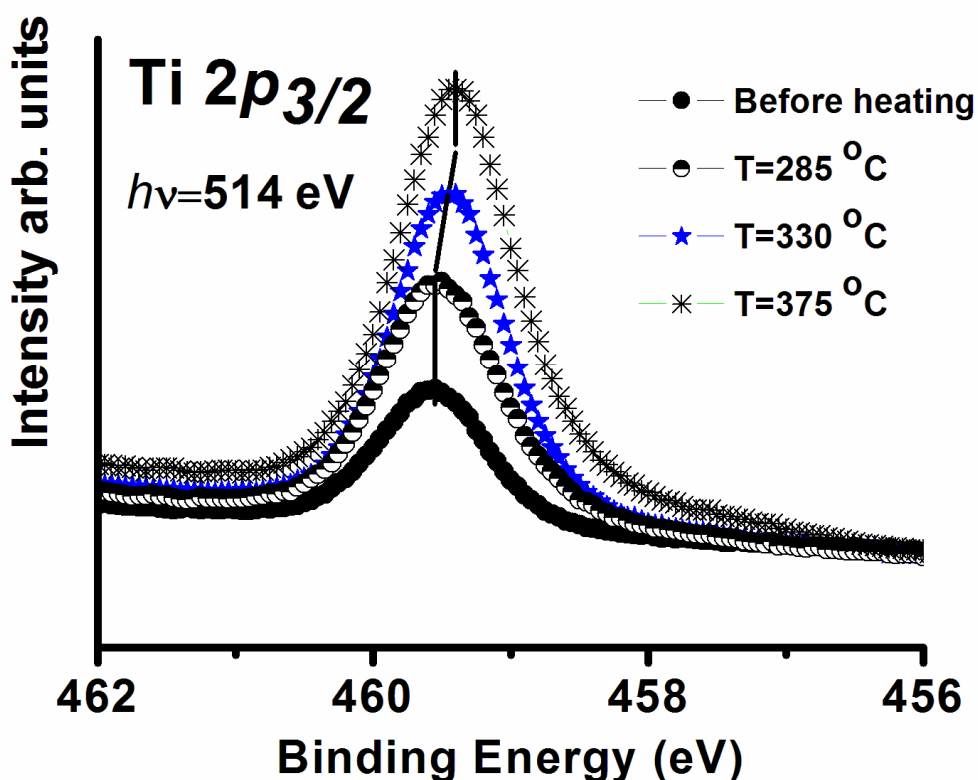


Fig. S2 Ti 2p photoelectron data. The Ti 2p_{3/2} spectra are shown using the relative intensities.

A shift of 0.13 eV, to lower binding energy, is observed at T= 330 °C and T= 375 °C, in contrast to the peak related to heating at T=285 °C. In addition, a comparison of the peak areas (calculated as the full width at half maximum, FWHM) before heating and after heating at T= 285 °C reveals that the increase in area of Ti 2p is around 34 %, a value in good agreement with the calculated decrease in area of C 1s at the same temperature (see Fig. 8 in the manuscript). The decrease in area for C 1s is related, in turn, to the amount of desorbed TBA⁺. The desorption of TBA⁺ does not affect the Ti 2p_{3/2} peak position since TBA⁺ is supposed to be physisorbed and not bonded to the TiO₂ surface as the dye does. The calculated areas for Ti 2p corresponding to T= 330 °C and T= 375 °C are, on the other hand, larger than what would be calculated amount of TBA⁺, and a shift is observed (see Fig. S1). The most plausible explanation is that decomposition and desorption of the ruthenium complex is taking place in these cases.