

New Approach of Modifying the Anatase to Rutile Transition Temperature in TiO₂ Photocatalysts

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Supplementary Information

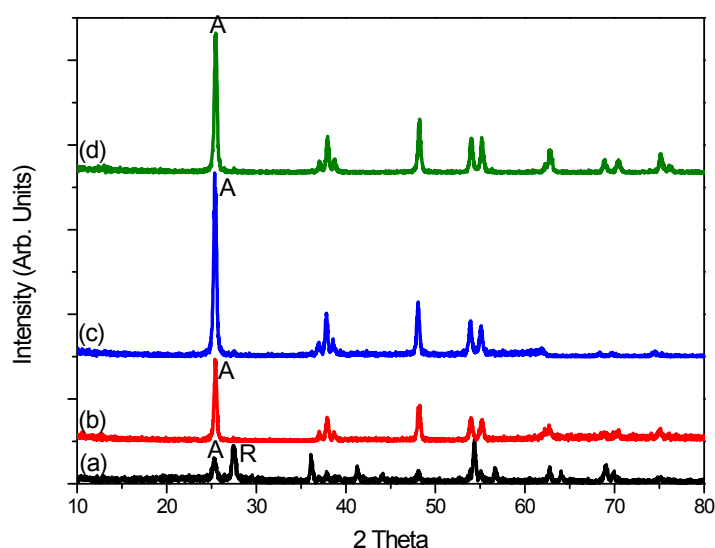


Figure S1: XRD of all concentrations that have been calcined at 600 °C. (a) Undoped TiO₂ (b) 1:1 TiO₂: Benzoic Acid (c) 1:4 TiO₂: Benzoic Acid and (d) 1:8 TiO₂: Benzoic Acid. A= anatase and R = rutile.

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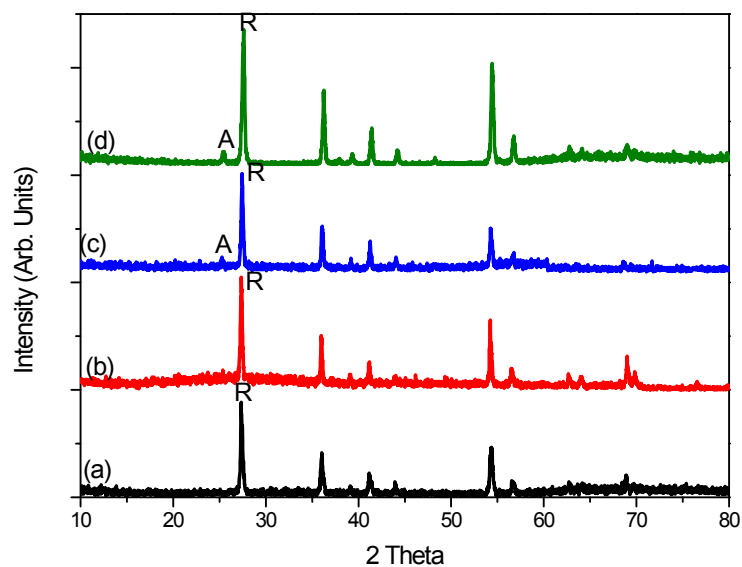


Figure S2: XRD of all samples which have been calcined at 800 °C. (a) Undoped TiO₂ (b) 1:1 TiO₂: Benzoic Acid (c) 1:4 TiO₂: Benzoic Acid and (d) 1:8 TiO₂: Benzoic Acid. A= anatase and R = rutile

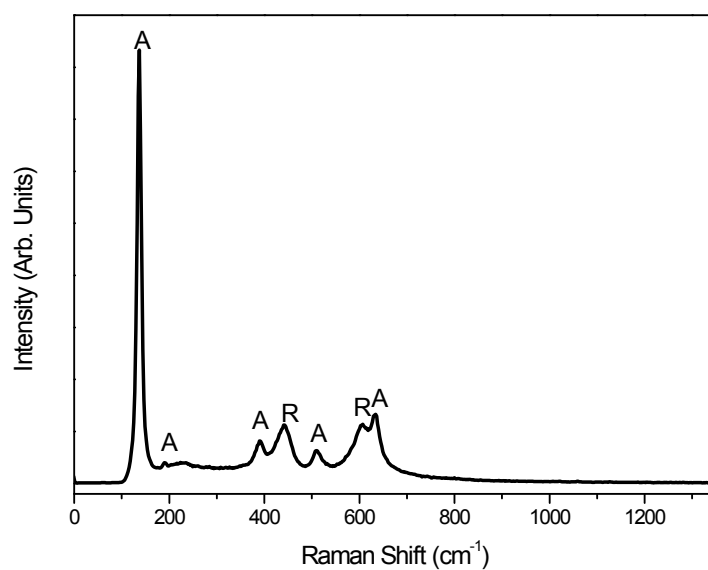
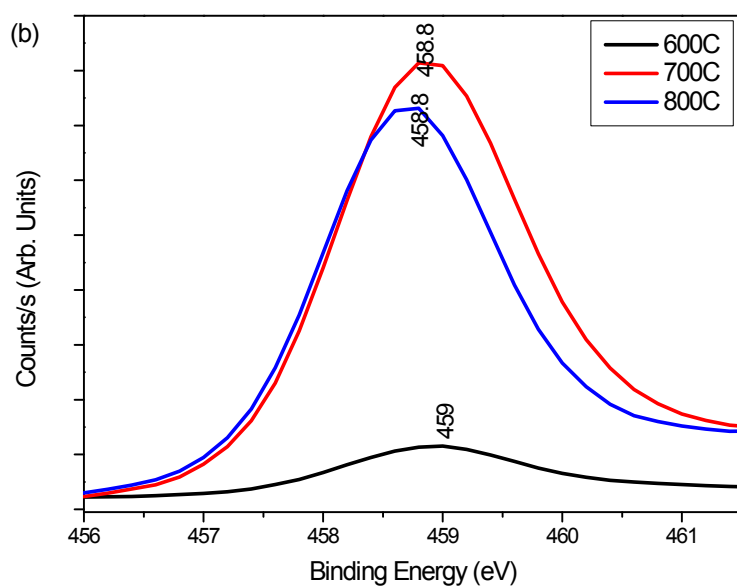


Figure S3: Raman spectra of the 1:1 TiO₂: benzoic acid sample calcined at 700 °C, A = anatase and R = rutile

Table S1: XPS results showing the binding energies (eV) for samples at 600 °C, 700 °C and 800 °C

	Control	1:1	1:4	1:8
C_{1s}	600 °C – 285.0	600 °C – 285.0	600 °C – 285.0	600 °C – 285.0
	700 °C – 285.0	700 °C – 285.0	700 °C – 285.0	700 °C – 285.0
	800 °C – 285.0	800 °C – 285.0	800 °C – 285.0	800 °C – 285.0
O_{1s}	600 °C – 530.2	600 °C – 530.2	600 °C – 530.2	600 °C – 530.0
	700 °C – 529.8	700 °C – 530.0	700 °C – 530.2	700 °C – 529.8
	800 °C – 530.0	800 °C – 529.8	800 °C – 530.0	800 °C – 529.8
Ti_{2p}	600 °C – 459.0	600 °C – 459.0	600 °C – 459.0	600 °C – 458.8
	700 °C – 458.8	700 °C – 458.8	700 °C – 458.8	700 °C – 458.6
	800 °C – 458.6	800 °C – 458.6	800 °C – 458.8	800 °C – 458.6

Figure S4: XPS of 1:4 TiO₂: benzoic acid at 600 °C, 700 °C and 800 °C for Ti_{2p 1/2}

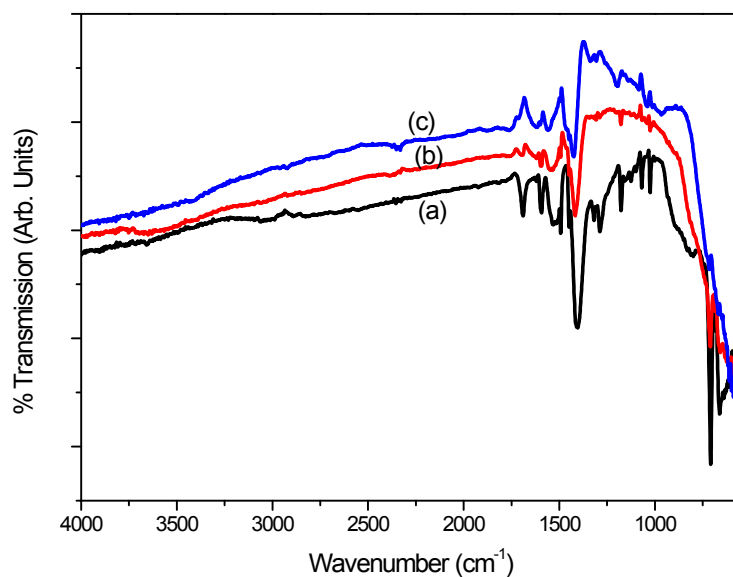


Figure S5: FTIR spectra of the 1:4 TiO₂: benzoic acid for (a) uncalcined, (b) 500 °C and (c) 900 °C

All 1:8 samples contained very weak Ti-O-Ti peaks, uncalcined at 556cm⁻¹, 500 °C at 530cm⁻¹ and 900 °C at 534cm⁻¹. The uncalcined and 500 °C samples both showed the presence of benzene ring(s), with a medium peak at 1036cm⁻¹ for uncalcined and a weak peak at 1025cm⁻¹ for the sample calcined to 500 °C. There is also a peak at 1287cm⁻¹ in the uncalcined sample for a carboxyl group (COOH) and one at 1319cm⁻¹ that indicates the presence of C-OH and is not present in the other samples. The uncalcined sample contains a strong C-O symmetric stretch (1403cm⁻¹), while 500 °C shows a medium C-O symmetric stretch (1416cm⁻¹) and at 900 °C a very weak C-O symmetric stretch (1427cm⁻¹). There are vibrations of carboxylate moieties at 500 °C (1538cm⁻¹). There are also peaks that show asymmetric C-O stretches, for uncalcined at 1590cm⁻¹ and 1690cm⁻¹ (medium) and for 500°C at 1590cm⁻¹ and 1690cm⁻¹ (weak).

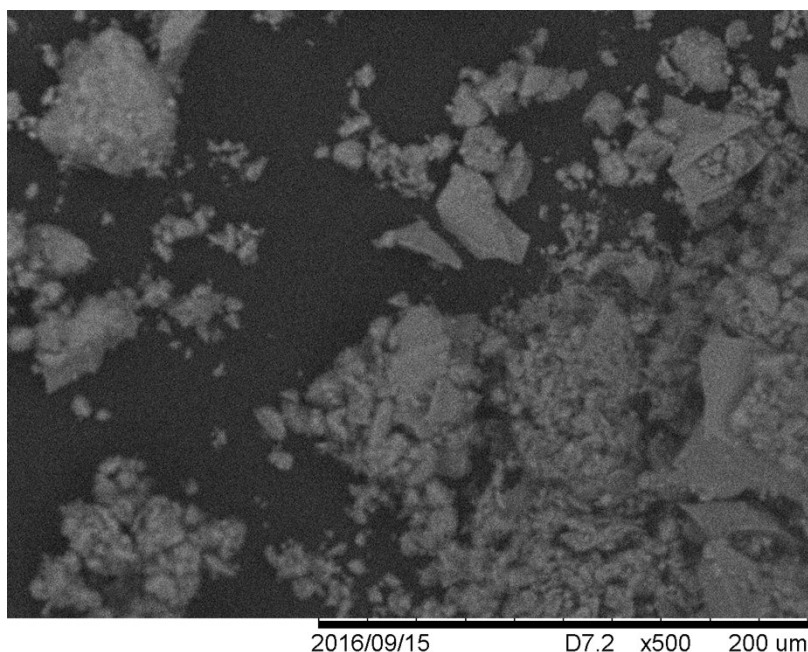


Figure S6: SEM of 1:4 TiO₂: benzoic acid @ 500°C