

Characteristics of the charge transfer surface complex on titanium (IV) dioxide for the visible-light induced chemoselective oxidation of benzyl alcohol

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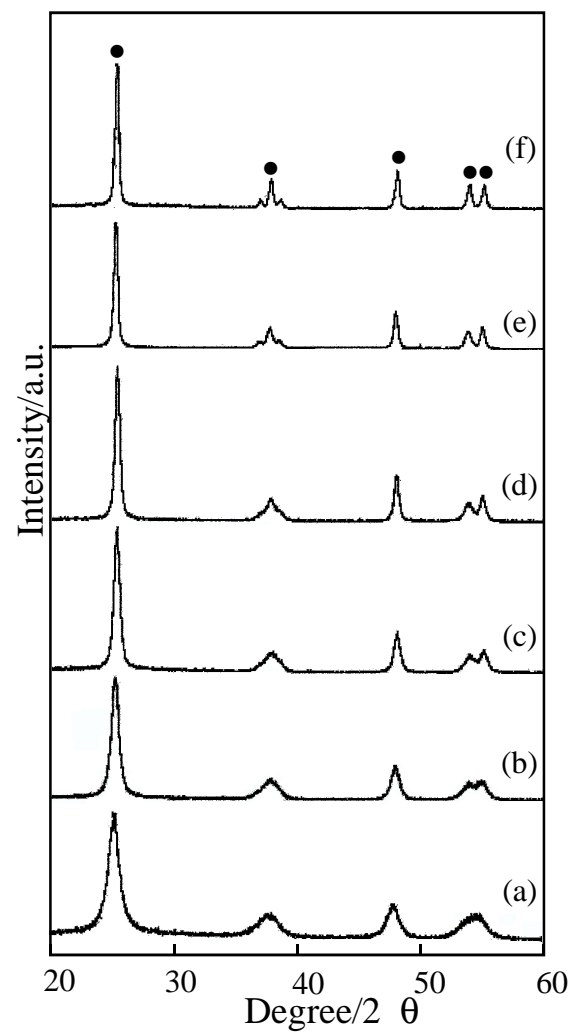


Figure S. 1 XRD patterns of (a) un-treated TiO_2 , (b) $\text{TiO}_2(573)$, (c) $\text{TiO}_2(673)$, (d) $\text{TiO}_2(773)$, (e) $\text{TiO}_2(873)$ and (f) $\text{TiO}_2(973)$. ●: anatase structure

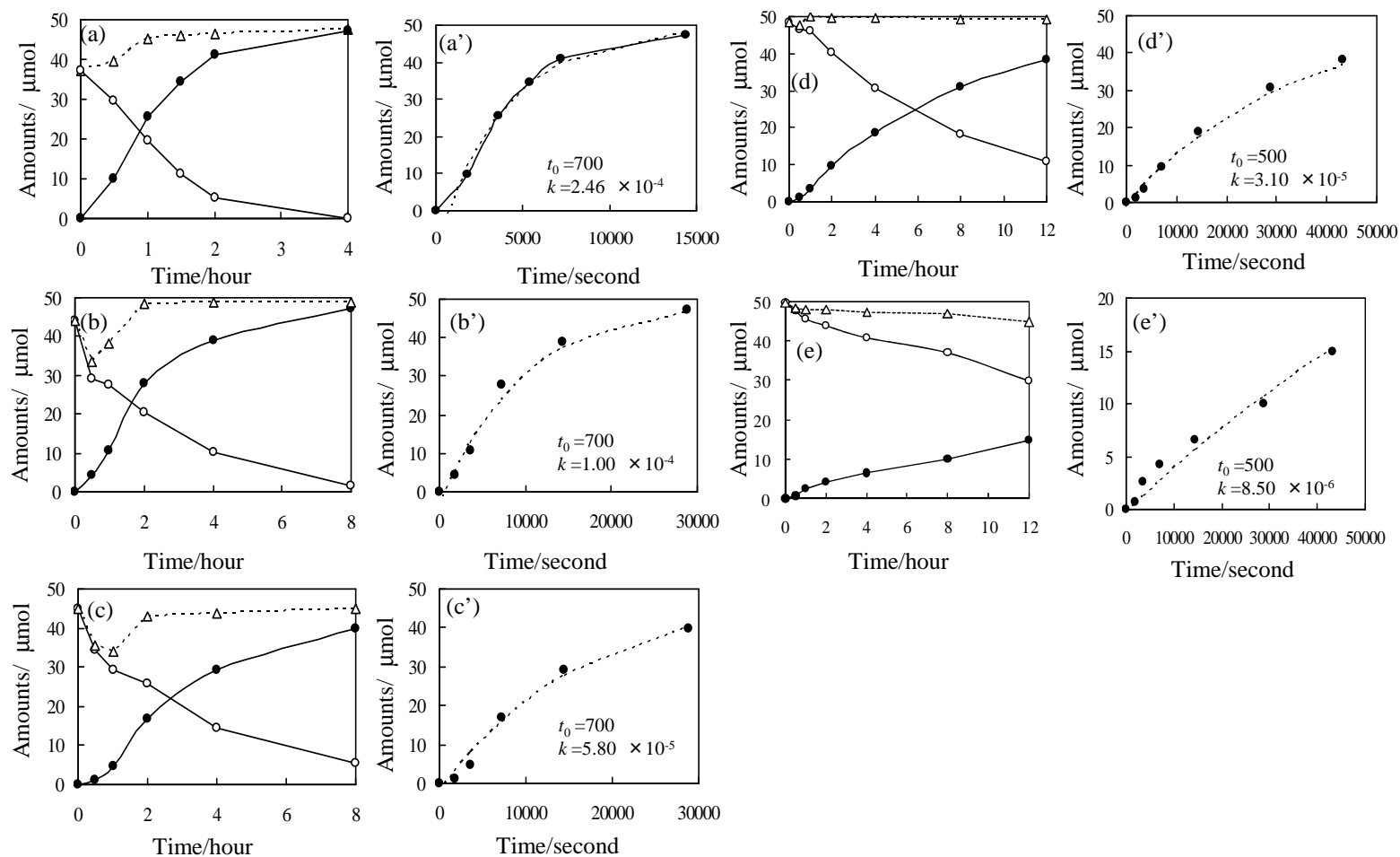


Figure S. 2 Time profile for the photocatalytic oxidation of benzyl alcohol on the heat-treated TiO₂ (a - e) in the presence of O₂ under visible light irradiation, and the simulation (broken line) of amounts of photo-formed benzaldehyde (a'-e'). a, a': un-treated TiO₂, b, b': TiO₂(673), c, c': TiO₂(773), d, d': TiO₂(873), e, e': TiO₂(973). \bullet : amount of benzaldehyde; \circ : amount of benzyl alcohol; Δ : amount of benzyl alcohol and benzaldehyde in total.

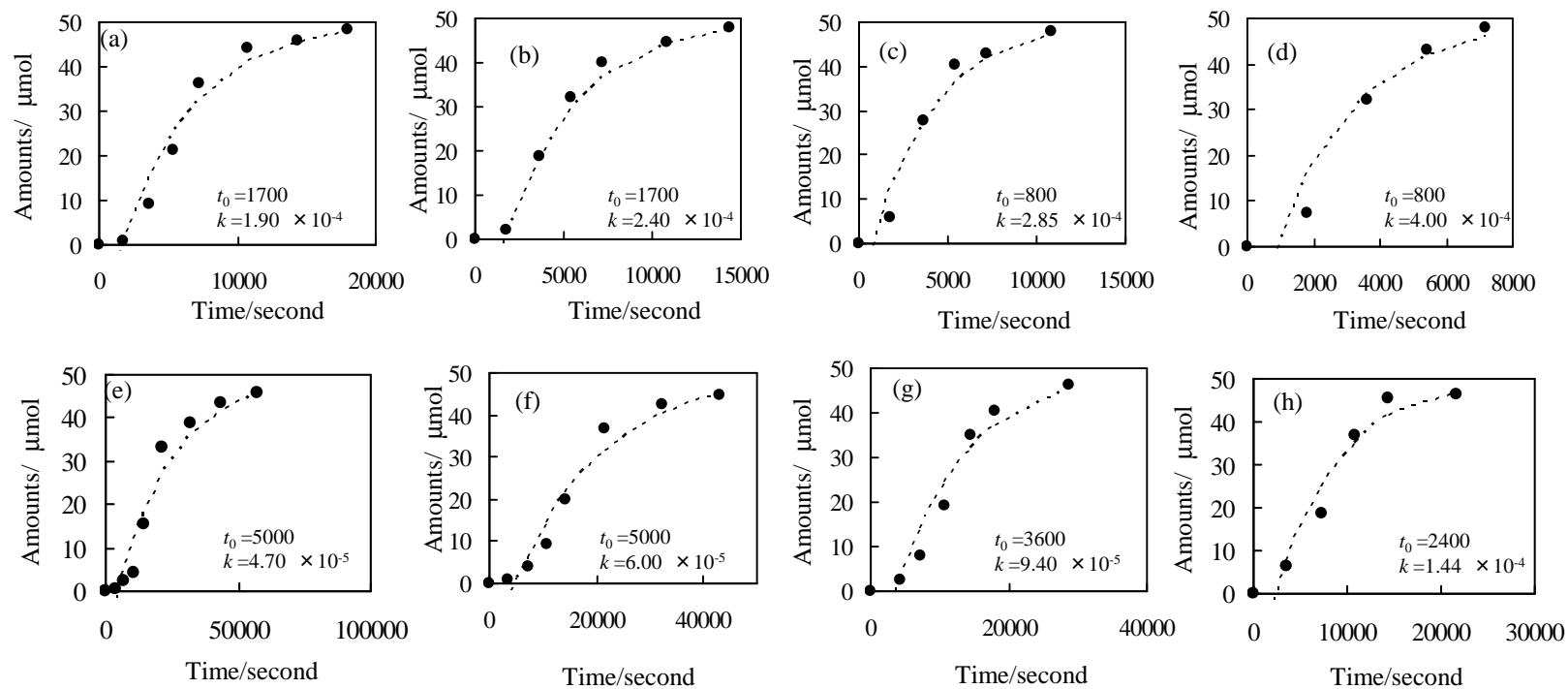


Figure S. 3 Time profile for the the photocatalytic oxidation of normal benzyl alcohol (a - d) and α , α -d2 benzyl alcohol (e - h) on TiO_2 with experiment (●) and its simulation (broken line). The reaction temperatures were controlled at 283 K (a, e), 293 K (b, f), 303 K (c, g) and 313 K (d, h).

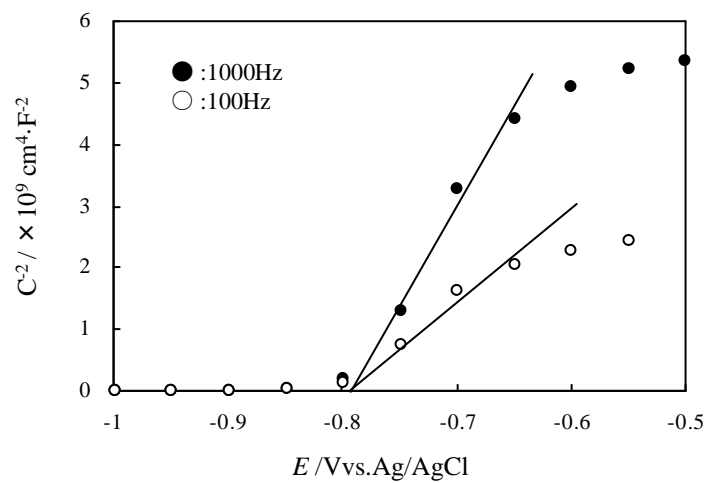


Figure S. 4 Mott-Schottky plots of the TiO_2 film electrode at the modulation frequency of 100 and 1000 Hz. The measurements were performed in acetonitrile solution involving 0.1 M LiClO_4 and 5 mM benzyl alcohol (pH = 3.8).

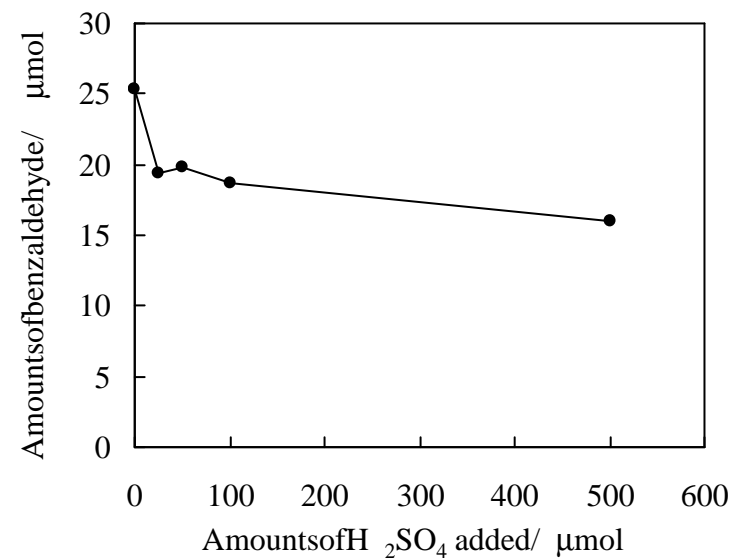


Figure S. 5 Plots for the amount of photo-formed benzaldehyde as a function of the amounts of conc. H₂SO₄ added. The photocatalytic oxidation of benzyl alcohol (50 µmol) was performed in acetonitrile solution on TiO₂ (50 mg) for 1h.