Electronic Supplementary Information for Dalton Transactions

Self-assembled TiO_2 nanoparticles: mesoporosity, optical and catalytic properties

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Supporting information

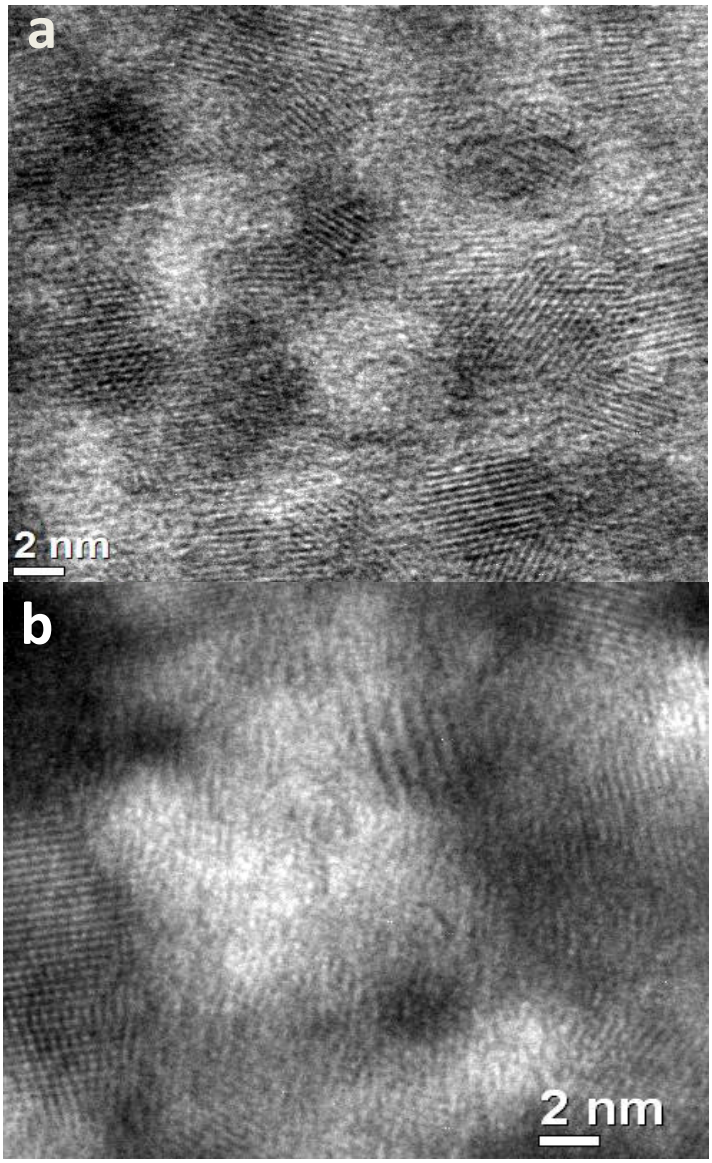


Figure S1: HRTEM images of self–assembled calcined mesoporous titania nanoparticles, synthesized by using SDS (sample 1, a) and F127 (sample 2, b) as templates and the pores that were created by assembly of titania nanoparticles. Seen through the direction perpendicular to the pore axis.

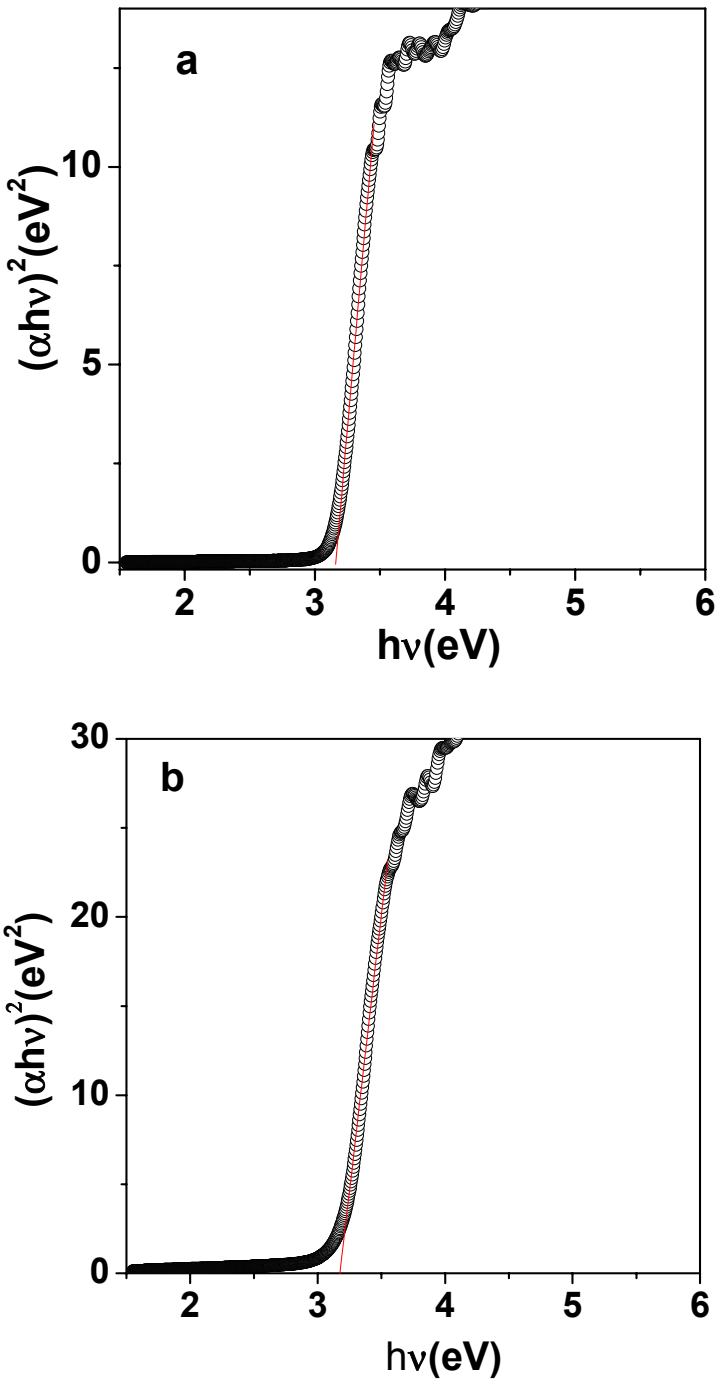


Figure S2: Band gap of calcined self–assembled mesoporous titania nanoparticles, synthesized by using SDS (a) and F127 (b) as templates

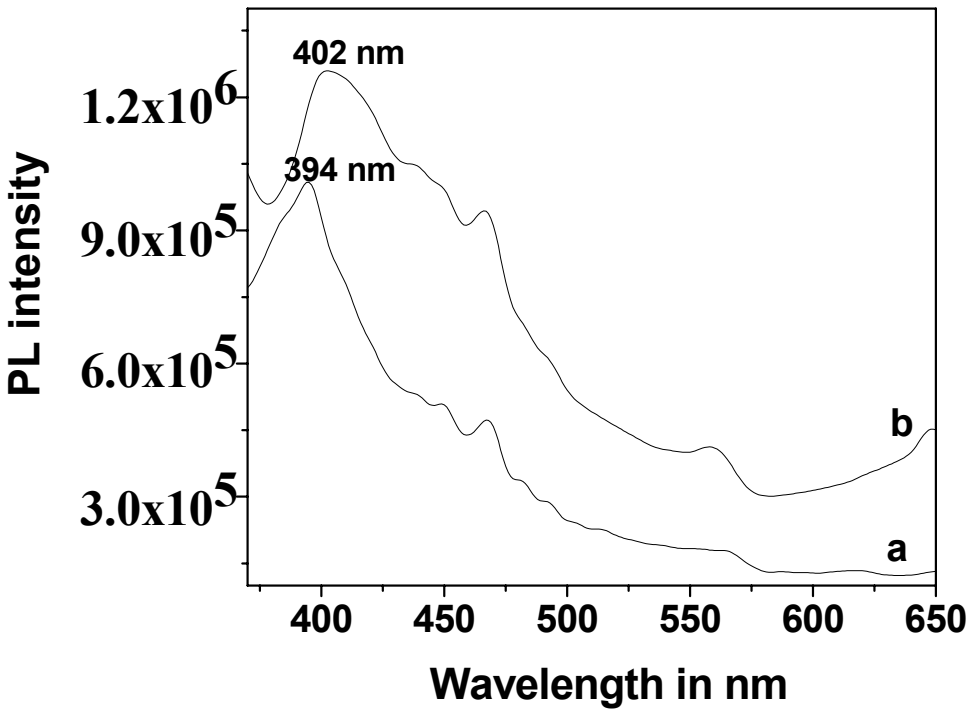


Figure S3: Photoluminescence spectra of self–assembled calcined mesoporous titania nanoparticles, sample 1 (a) and sample 2 (b).

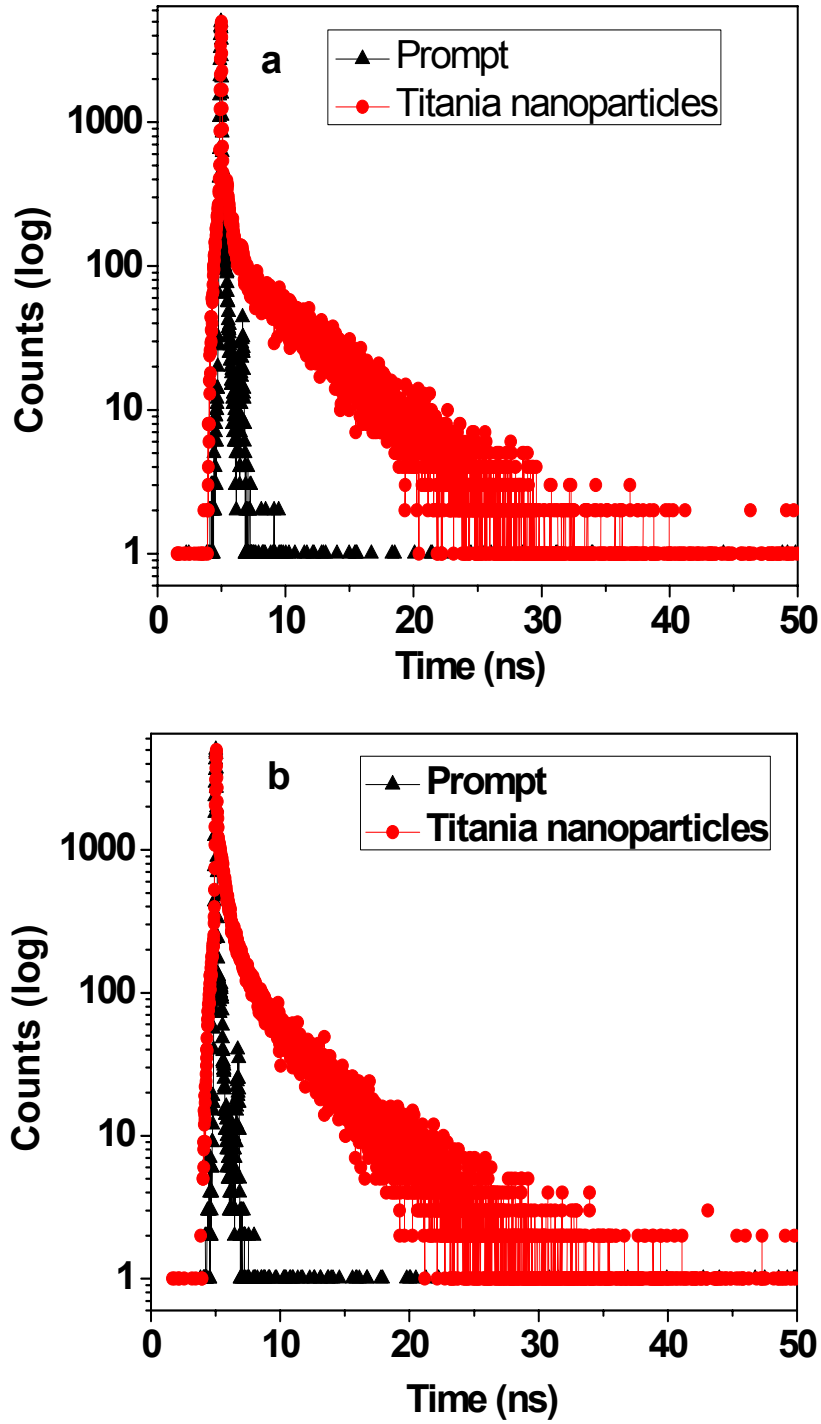


Figure S4: Time resolved fluorescence decay profiles of self–assembly calcined mesoporous titania nanoparticles, sample 1 (a) and sample 2 (b). Fluorescence lifetimes were determined by the time-resolved intensity decay method of time-correlated single-photon counting (TCSPC) by using a Horiba Jobin Yvon Fluoro Cube instrument with an excitation wavelength of 350 nm from a Diode Laser.

Table S1. Emission maximum, component of emission lifetime (τi) and the preexponential factor (αi)[a] for the decays corresponding as–synthesized and calcined mesoporous titania nanoparticles.

Sample type	Emission maximum (nm)	τ_1 (ns)	τ_2 (ns)	τ_3 (ns)	χ^2	τ_{av} (ns)
Calcined mesoporous titania using SDS (sample 1)	390	0.526 (15.59)	5.095 (38.50)	0.033 (46.01)	1.09	4.59
Calcined mesoporous titania using F127 (sample 2)	396	0.0068 (55.14)	0.574 (22.15)	4.191 (22.71)	1.096	5.269

a: Preexponential factors for each component are given in parentheses.

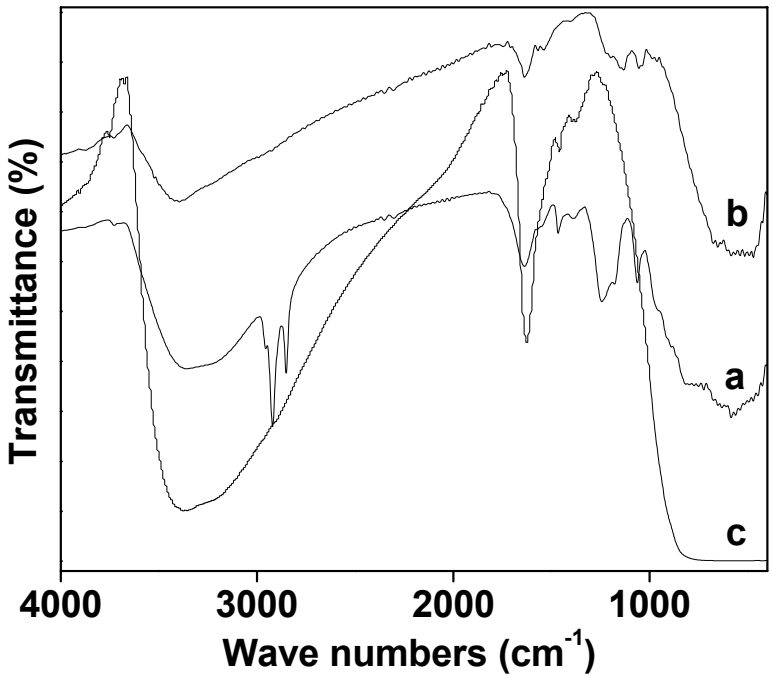


Figure S5: FT–IR spectra of self-assembled as–synthesized (a), calcined (b) sample 1 and calcined bulk titania material (c).

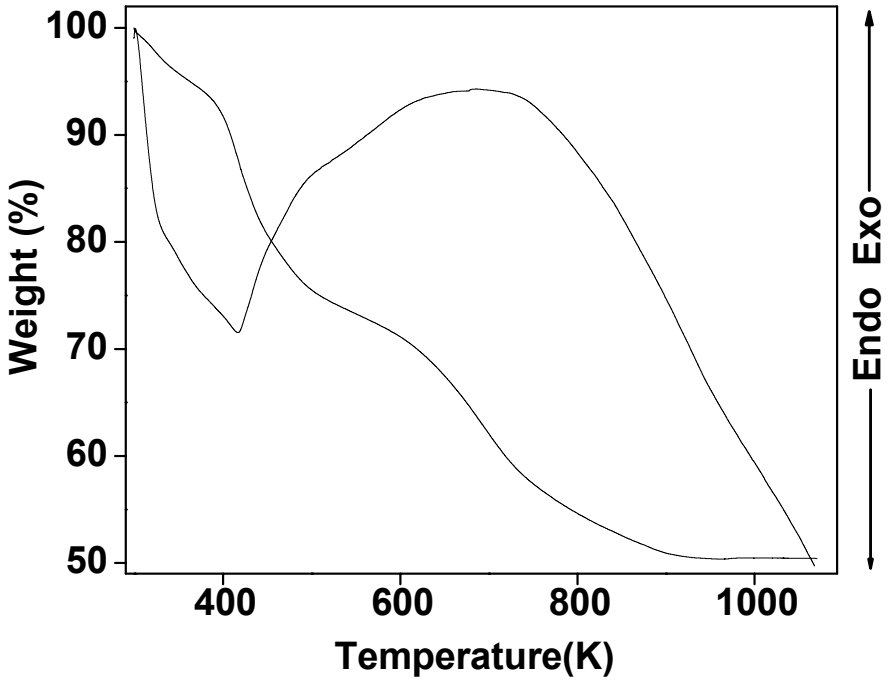
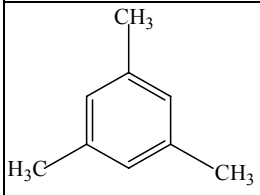
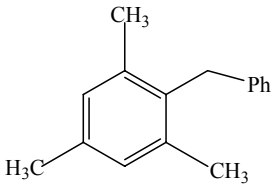
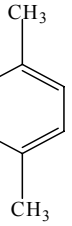
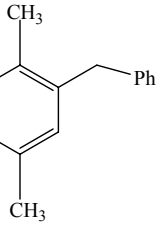
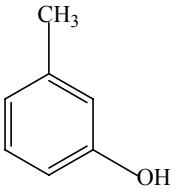
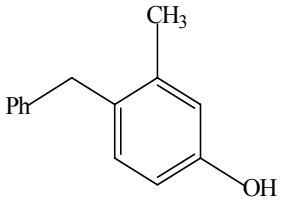
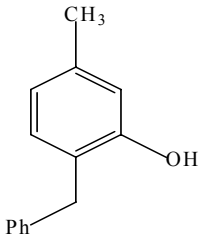
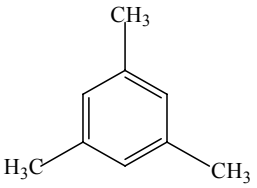
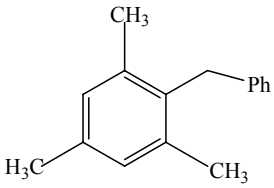


Figure S6: TGA, DTA of as–synthesized mesoporous titania nanomaterials (sample 1, as representative).

Table S2. Benzylation reactions catalyzed by mesoporous titania at 348 K

Substrate	Product	MRS: BC[a]	Time (h)	Conversion (%)	Selectivity (%)	TON[b]
		10:1	12	83.02	100	4.85
		10:1	12	82.19	100	5.41
	 and 	10:1	9	98.41	65.77 (major) 34.23 (minor)	6.47
		10:1	12	1.7	89.02[c]	—

a: Mole ratio of substrate and benzyl chloride. b: Moles of substrate converted per mole of titania site present in the catalyst. c: Reaction was carried out in absence of any catalyst.

d: Since large excess of different aromatic compounds have been taken in these reactions percentage of conversion was estimated by taking benzyl chloride as standard.