Supporting information

Revealing the Structural Properties of Hydrogenated Black TiO₂ Nanocrystals

Ting Xia¹, Xiaobo Chen^{1,*}

¹Department of Chemistry, University of Missouri – Kansas City, Kansas City, MO 64110, U.S.A. Detailed XRD analysis data

Peak	Angle / degree		FWHM / degree		Plane distance / Å		Directional size / Å	
index	white	black	white	black	white	black	white	black
	TiO ₂	TiO ₂	TiO ₂	TiO ₂				
101	25.21	25.32	0.98	1.04	3.533	3.517	83.131	78.352
004	37.82	37.89	1.31	1.33	2.379	2.374	64.153	63.202
200	48.00	48.08	1.11	1.15	1.895	1.892	78.404	75.701
105	53.87	54.08	0.99	1.01	1.702	1.696	90.080	88.378
211	54.89	55.07	1.05	1.04	1.673	1.668	85.321	86.212
204	62.50	62.67	1.43	1.22	1.486	1.482	65.033	76.296
116	68.81	68.85	1.07	1.32	1.364	1.364	90.058	73.019
220	70.13	70.43	1.30	1.31	1.342	1.337	74.719	74.285
215	75.23	75.27	1.26	1.67	1.263	1.262	79.657	60.117

Table S1. Size of pure and hydrogenated TiO₂ nanocrystals derived from XRD data.

Table S2. Unit cell parameters of pure and hydrogenated TiO_2 nanocrystals derived from XRD data.

	Cell parameter a / Å	Cell parameter c / Å	Cell volume / Å ³	Surface excess pressure / GPa	Surface stress / N/m
Bulk TiO ₂	3.789	9.537	136.93	0	0
White TiO ₂	3.791	9.515	136.72	0.276	0.557
Black TiO ₂	3.785	9.498	136.05	1.157	0.532

Table S3. Sur	face area and surfa	ace percentage o	f different facet	s of white a	nd black	TiO_2
nanocrystals.						

Facet	Surface	area/nm ²	Surface percentage		
	white TiO ₂	black TiO ₂	white TiO ₂	black TiO ₂	
001	20.457	9.731	0.113	0.0647	
100	6.438	8.173	0.036	0.0544	
110	31.774	7.128	0.175	0.0474	
102	122.399	0	0.676	0	
215	0	125.276	0	0.8335	

Comparison of the crystal morphology model with the HRTEM images of pristine white

TiO₂ nanocrystals.



Comparison of the crystal morphology model with the HRTEM images of hydrogenated black TiO_2 nanocrystals.



Comparison of the crystal morphology model with the HRTEM images of hydrogenated black TiO_2 nanocrystals.

