

## Supporting Information

### Controlled Synthesis of Linear and Branched Au@ZnO Hybrid Nanocrystals and Their Photocatalytic Properties

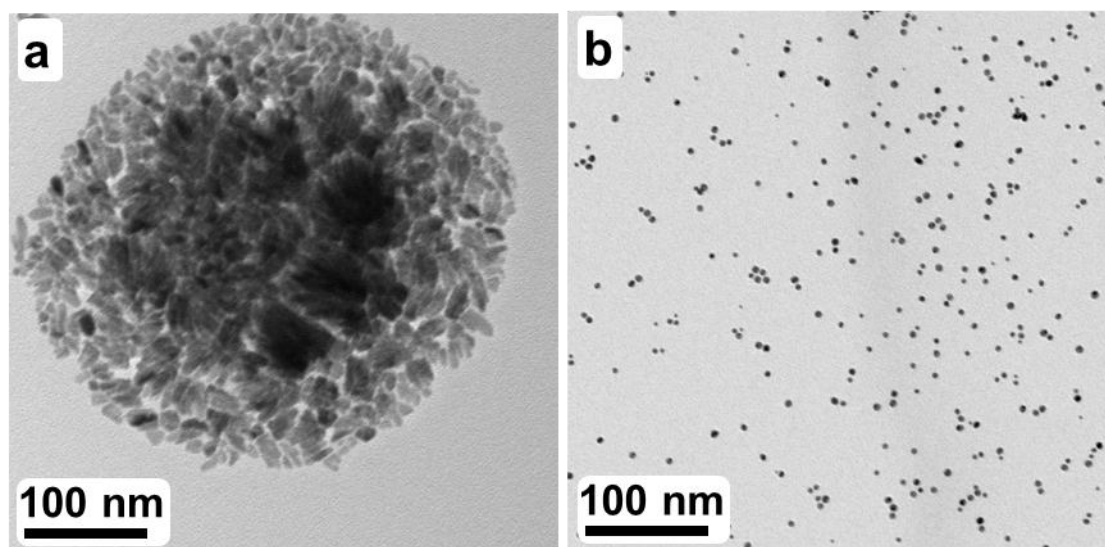
Muhammad Nawaz Tahir<sup>a\*</sup>, Filipe Natalio<sup>a†</sup>, Musa Ali Cambaz<sup>a</sup>, Martin Panthöfer<sup>a</sup>, Robert Branscheid<sup>b</sup>, Ute Kolb<sup>b</sup>, Wolfgang Tremel<sup>a\*</sup>

*Received (in XXX, XXX) Xth XXXXXXXXXX 20XX, Accepted Xth XXXXXXXXXX 20XX*

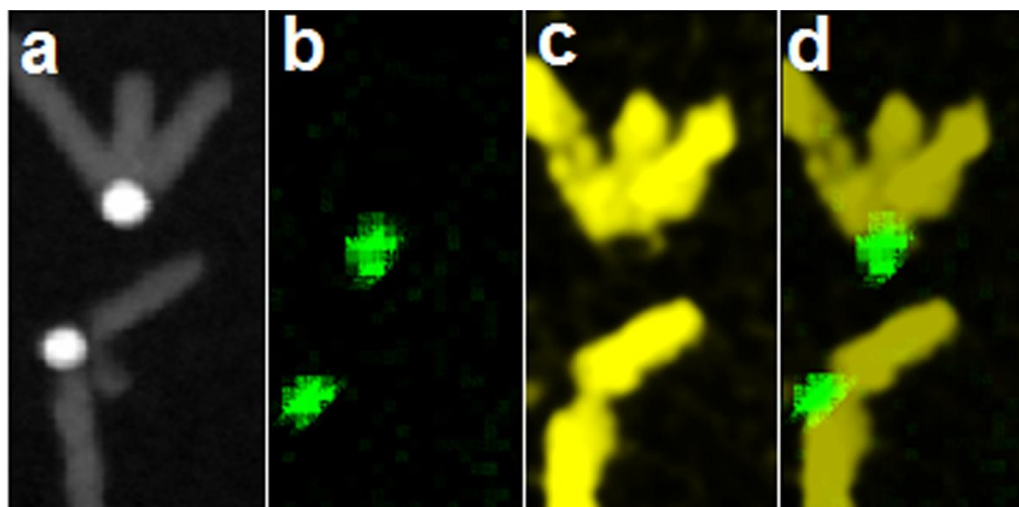
DOI: 10.1039/b000000x

**Table S1.** Details of the measurement and refinement of the x-ray diffraction data.

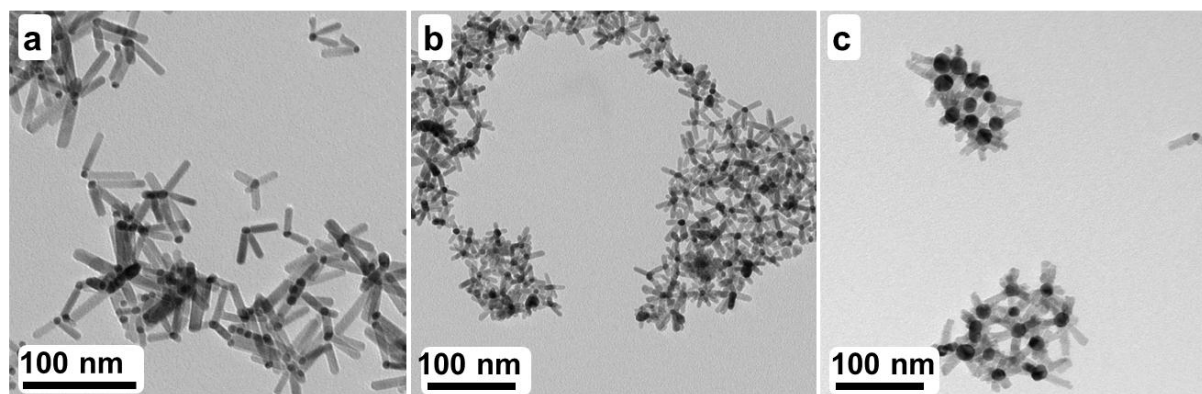
	<b>ZnO nanorods</b>	<b>linear Au@ZnO</b>	<b>branched Au@ZnO</b>
Diffractionmeter	Siemens D5000, Ge- monochromator, Braun M50 PSD		
Sample preparation	Thin powder layer between two Scotch magic adhesive tape strips		
Measuring mode	Transmission		
Wavelength	CuK $\alpha_1$ , 1.540596Å		
Measuring range	1407 $\leq 2\Theta /^\circ \leq 75.7$ , $\Delta 2\Theta /^\circ = 0.039$ , 6sec/step; $1 \leq Q/\text{\AA}^{-1} \leq 5.0$ Sum of three individual scans for improving S/N ratio		
Temperature /K	298		
Profile Fit	Rietveld refinement according to reported crystal structure models		
Background / Parameters	Chebyshev / 12	Chebyshev / 18	
Profile function	Fundamental Parameters Approach, enhanced for modelling anisotropic crystallite morphology		
Program	TOPAS Academic V4.1		
Total No. of Parameters	20	24	24
R <sub>wp</sub>	4.98	5.85	4.48
GoF	2.02	2.44	1.81
<b>Phase I</b>	<b>ZnO, Zincite</b>		
Space group	<i>P6<sub>3</sub>mc</i>		
Cell parameters /Å	a = 3.2431(3) c = 5.1992(5)	a = 3.2471(3) c = 5.2024(6)	a = 3.2475(3) c = 5.2036(6)
Crystallite size / nm	20(1) by 58(1)	19(1) by 70(2)	18(1) by 76(2)
Fraction /%wt	100	83.4(6)	81.9(5)
Biso	1.0	1.0	1.0
Preferred Orientation (March-Dollase)	(110) / 0.966(7)	(110) / 0.980(7)	(110) / 1.00(1)
<b>Phase II</b>	<b>Au, Gold</b>		
Space group	<i>Fm-3m</i>		
Cell parameters /Å		a = 4.040(1)	a = 4.058(1)
Crystallite size / nm		5(1)	6(1)
Fraction /%wt		16.6(4)	18.1(5)
Biso		1.0	1.0
Preferred Orientation (March-Dollase)		(111) / 0.626(9)	(111) / 0.70(1)



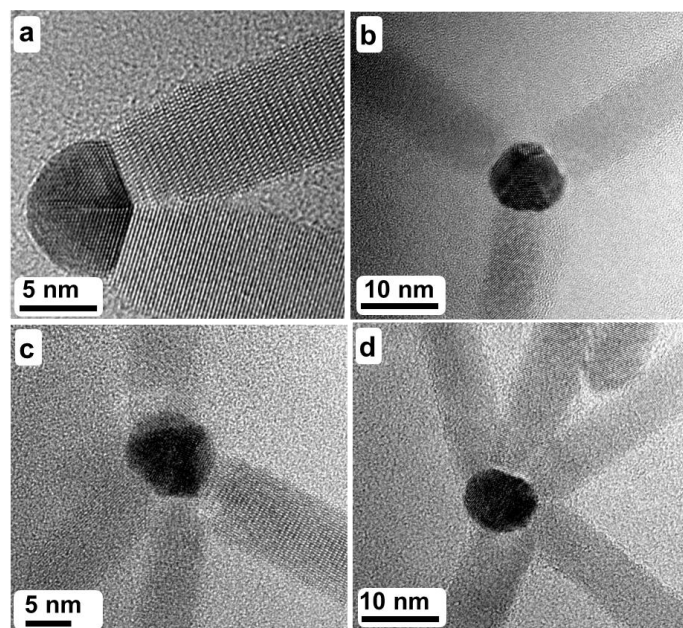
**Fig. S1.** (a) Overview TEM image of ZnO nanoparticles synthesized in benzyl alcohol and (b) overview TEM image of Au nanoparticles taken from the reaction flask at 120° C.



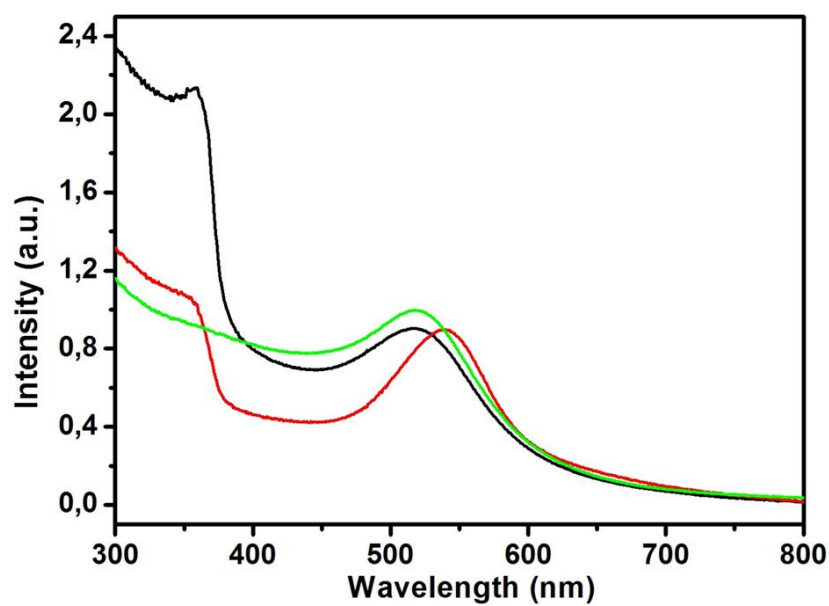
**Fig. S2.** Elemental mapping of branched Au@ZnO nanoparticles synthesized in benzyl alcohol. (a) STEM mode image and corresponding elemental maps of (b) Au (green), and (c) Zn (yellow) as well as an overlay image (d) obtained by recording the spatial distributions.



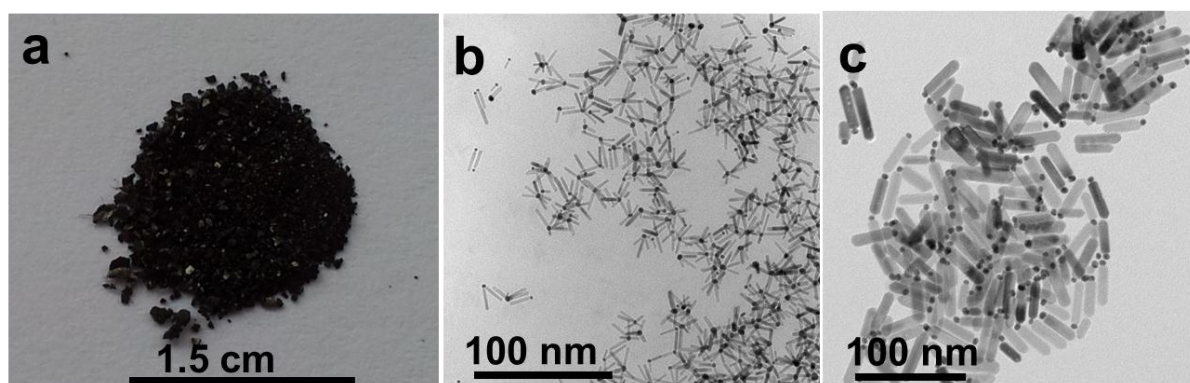
**Fig. S3.** TEM images of the branched Au@ZnO hybrid nanocrystals synthesized with (a) 20 mg (0.1 mmol) of  $\text{HAuCl}_4 \cdot x\text{H}_2\text{O}$  and 109 mg (0.5 mmol) of  $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ , (b) 20 mg (0.1 mmol) of  $\text{HAuCl}_4 \cdot x\text{H}_2\text{O}$  and 60 mg (0.25 mmol) of  $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ , (c) 40 mg (0.2 mmol) of  $\text{HAuCl}_4 \cdot x\text{H}_2\text{O}$  and 109 mg (0.5 mmol) of  $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ , respectively.



**Fig. S4.** HRTEM images of the branched Au@ZnO hybrid nanocrystals with different numbers of ZnO nanorods on Au seed nanocrystals.

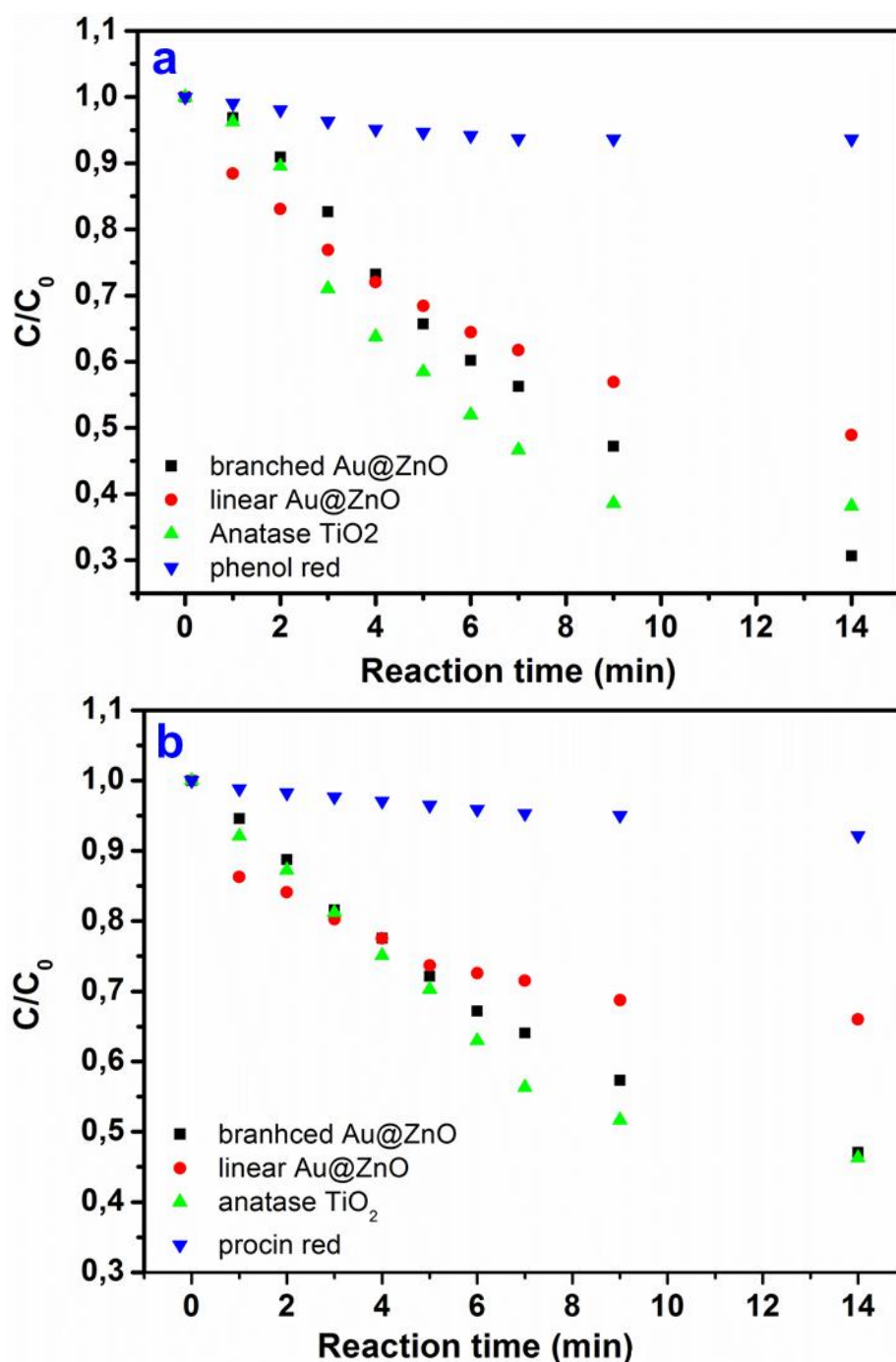


**Fig. S5.** UV-vis spectra of the branched Au@ZnO hybrid nanocrystals synthesized with 0.1 mmol Au precursor and 0.5 mmol of Zinc acetate dihydrate (black line), 0.2 mmol of Au and 0.5 mmol of Zinc acetate dihydrate precursors (black line), respectively. The UV-vis spectrum (green line) corresponds to Au aliquots of nanoparticle taken at 120° C from the reaction flask.

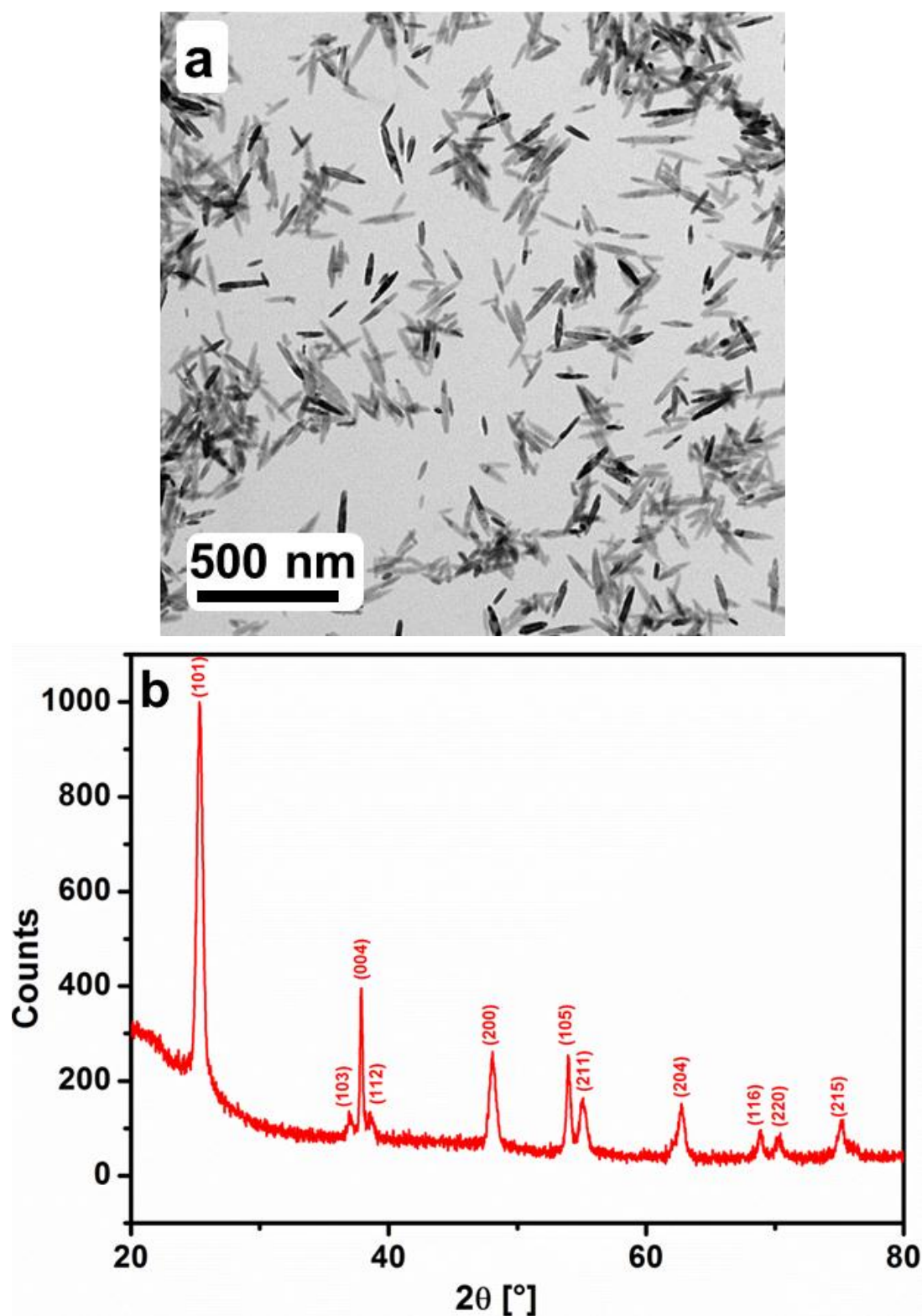


**Fig. S6.** (a) photograph showing almost 1g of Au@ZnO heterodimer nanocrystals. (b & c) corresponding TEM images of the 5 times upscaled synthesis of branched and linear shape Au@ZnO heterodimers respectively.





**Fig. S7.** a) Kinetic profile of photocatalytic degradation of phenol red (0.5 mg/mL) under UV irradiation (500W, total exposure time of 14 min) in the presence of imidazole-functionalized branched (black squares) and linear (red spheres) Au@ZnO hybrid nanocrystals. As synthesized anatase TiO<sub>2</sub> nanorods (green triangles) and phenol red (0.5 mg/mL) (blue triangles) solutions were used as control. The phenol red degradation was monitored at  $\lambda = 559,18$  nm. b) Kinetic profile of photocatalytic degradation of procin red (0.5 mg/mL) under UV irradiation (500W, total exposure time of 14 min) in the presence of imidazole-functionalized branched (black squares) and linear (red spheres) Au@ZnO hybrid nanocrystals. As synthesized anatase TiO<sub>2</sub> nanorods (green triangles) and procin red (0.5 mg/mL) (blue triangles) solutions were used as control. The RhB degradation was monitored at  $\lambda = 536,56$  nm.



**Fig. S8.** (a) Overview TEM image of as synthesized TiO<sub>2</sub> nanorods. (b) X-ray diffraction pattern of as synthesized TiO<sub>2</sub> nanorods. The pattern can be fully indexed to anatase.