Electronic Supplementary Material (ESI) for RSC Advances.

Visible-light photocatalytic performances of TiO_2 nanobelts decorated with iron oxide nanocrystals

Supporting information

Phase analysis

The estimation of the percent of Fe_2O_3 in the produced TiO_2-Fe_2O_3/Ti heterostructure was achieved by X-ray diffraction analysis (Fig. SI-1). Chemical analysis of Fe and Ti elements was not used for such a purpose since it did not allow a rigorous quantification of the different constituting crystalline phases. Indeed, Ti atoms exist in both metal and metal oxide crystals.

Rietveld refinement usually gives the quantification of each constituting crystalline phase (weight ratio). The accuracy is usually less than 10% and it is improved when the quality of the recorded pattern is high. Typically, patterns recorded in θ-θ conditions on samples made from strain free, large (micrometer-sized) and isotropic in shape crystals give the best results.

In this study, we prepared TiO_2 NBs and we decorated them by Fe_2O_3 NCs to improve their properties to serve as efficient photocatalyts and/or photoelectrocatalysts. We recorded the XRD pattern of the resulting hybrid in grazing conditions to enhance the diffraction signal of the surface sample. We observed diffractions lines matching very well with those of hematite, anatase (major), rutile (minor) and α-Ti crystalline phases, the contribution of the formers being overestimated compared to that of the latter. The Fe_2O_3 diffraction lines are broadened, not always well-resolved and of a very low intensity compared to those of the other surface phases, making the quantification analysis more or less delicate. As a first approximation a hematite weight content of 28 % was obtained (Table SI-1).

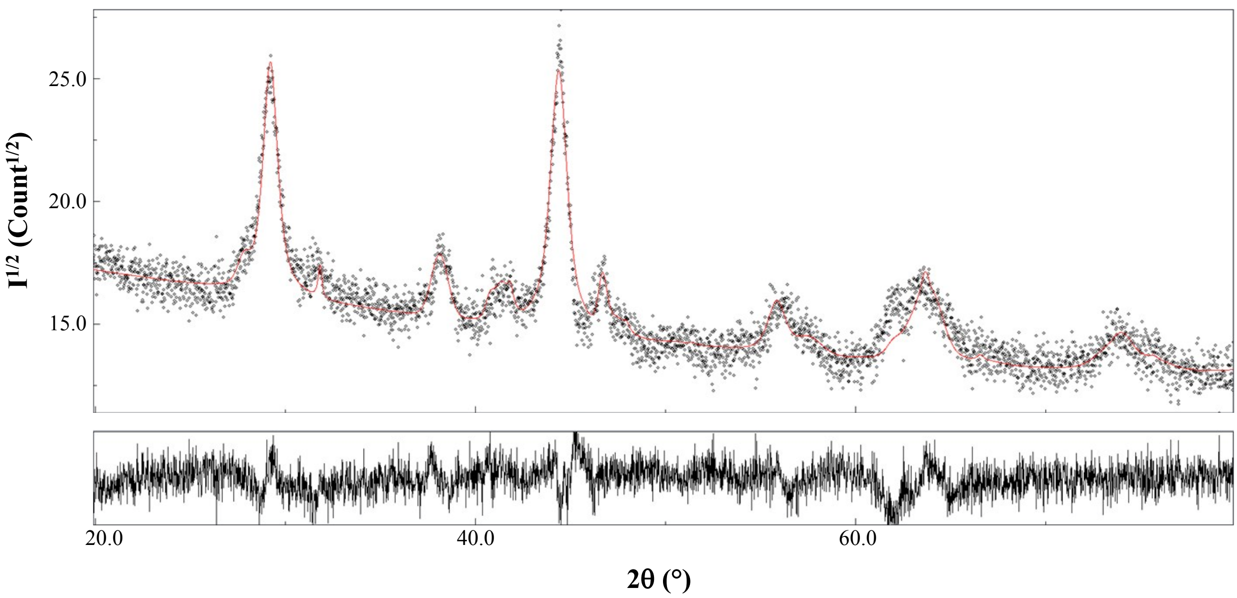

Figure SI-1. Experimental XRD pattern of the produced semiconducting heterostructure (scatters) superposed to the calculated one (red line). The difference between them (bold black line) is given ti appreciate the fit quality.

Hematite (wt.-%)	α-Ti (wt.-%)	Anatase (wt.-%)	Rutile (wt.-%)
24 (±2)	9 (±1)	64 (±4)	3 (±1)

Table SI-1. Weight content of the different constituting crystallographic phases of the TiO_2-Fe_2O_3/Ti heterostructure as inferred from grazing X-ray diffraction analysis using HIGHSCORE+ software (PANALYTICAL). These values were obtained for a GOF parameter of 1.22.

Optical analysis

The band gap (E_g) values of TiO_2/Ti and TiO_2-Fe_2O_3/Ti were estimated using the Tauc equation and starting from the UV-vis absorption data, assumin indirect gap semiconductors: [1]

$(F(R) \times h\upsilon) = k \times (h\upsilon\text{-}Eg)^{1/2}$

In practice, the linear portion of the $(F(r).hv)^{1/2}$ versus hv curves is extrapolated to the X-axis and the intersection point measures E_g (Fig. SI-2).

In these conditions a direct determination of the average bandgap value of the TiO_2-Fe_2O_3/Ti hybrid is possible. A value of 2.7 eV, smaller than that measured on bare TiO_2/Ti (3.2 eV), is found, in agreement with the attachment on the wide bandgap TiO_2 semiconductors of narrow bandgap Fe_2O_3 ones.

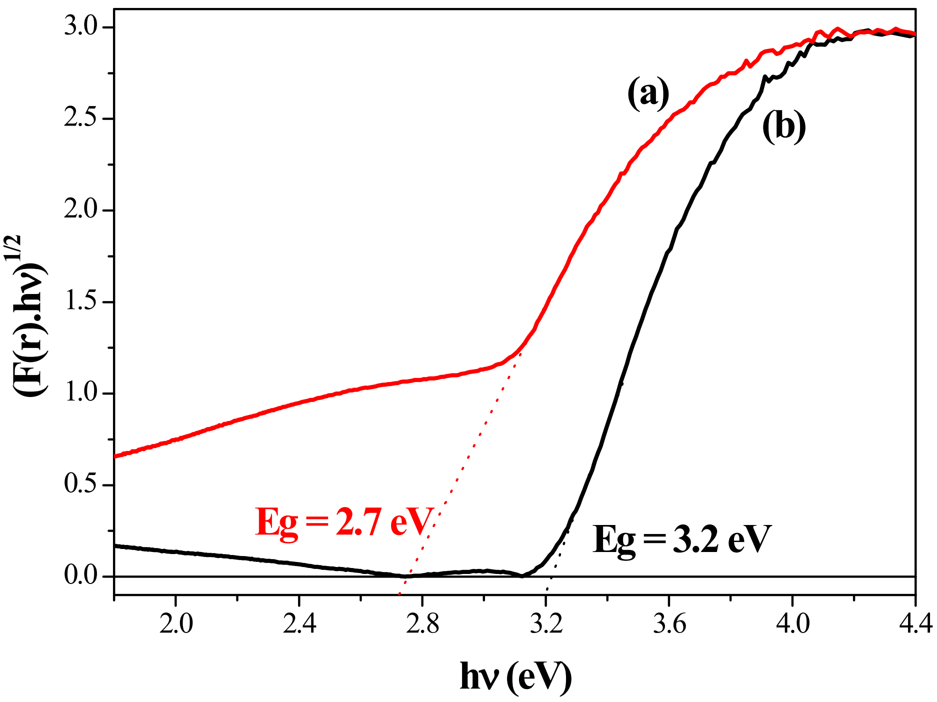

Figure SI-2. Determination of the optical band gap of TiO_2-Fe_2O_3/Ti (a) and TiO_2/Ti and nanostructures by Tauc plot.

[1] Y. Zhou, A. Wang, Z. Wang, M. Chen, W. Wang, L. Sun and X. Liu, Titanium functionalized α-zirconium phosphate single layer nanosheets for photocatalyst applications, *RSC Adv.,* 2015, 5, 93969–93978.